Uvod u atomsku mehaniku II

(31 - 66)

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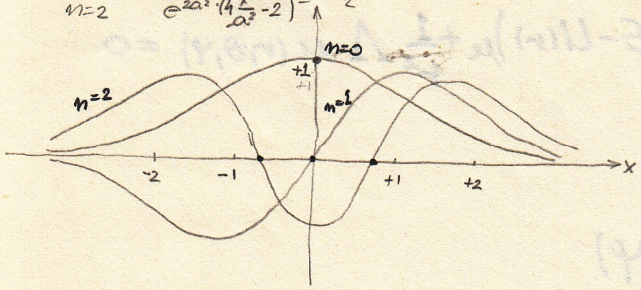
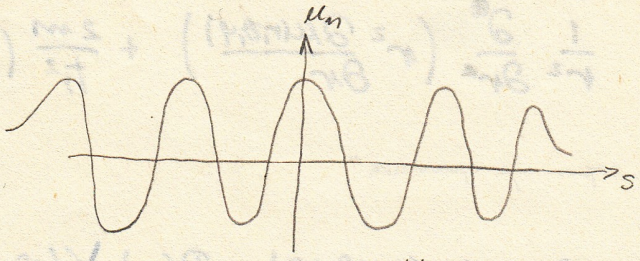
$n=0$ $e^{-\frac{x^2}{2a^2}} \cdot 1 = u_0$

$n=1$ $e^{-\frac{x^2}{2a^2}} \cdot 2\frac{x}{a} = u_1$

$n=2$ $e^{-\frac{x^2}{2a^2}} \cdot (4\frac{x^2}{a^2} - 2) = u_2$

n - broj čvorišta





približno kao ravni val

Schröd. jba. za 3-Dim. slučaj

- već za 1-Dim. slučaj je klasa potencijala strogo ograničena, gdje se može dobiti analitičko rješenje

Pojednostavljeni tipovi:

- promatramo kada se može učiniti separacija dif. jbe.

1) $U(x,y,z) = U_x(x) + U_y(y) + U_z(z)$ $\quad \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + (E - U_x(x))\right]u = 0$

$\rightarrow u(x,y,z) = u_x(x) + u_y(y) + u_z(z)$

i jbe: $\frac{d^2u_x}{dx^2} + \frac{2m}{\hbar^2}(E_x - U_x)u_x = 0$

$\vdots$

gdje je $E_x + E_y + E_z = E$

↑ 3 nove konst.

!!! koncept

neovisna x, y, z titranja

2) Sfernosimetrični potencijali

$U = U(r)$

Laplace-ov operator

$$\Delta u = \underbrace{\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial u}{\partial r}\right)}_{\frac{1}{r}\frac{\partial^2}{\partial r^2}(ru)} + \frac{1}{r^2}\Lambda u$$

$$\Lambda u = \frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial u}{\partial\vartheta}\right) + \frac{1}{\sin^2\vartheta}\frac{\partial^2 u}{\partial\varphi^2}$$

$\frac{1}{r}\frac{\partial^2}{\partial r^2}(r\cdot u(r,\vartheta,\varphi))$

$$\Rightarrow \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial u(r,\vartheta,\varphi)}{\partial r}\right) + \frac{2m}{\hbar^2}(E-U(r))u + \frac{1}{r^2}\Lambda u(r,\vartheta,\varphi) = 0$$

„separacija operatora"

$$\rightarrow \quad u(r,\vartheta,\varphi) = R(r)\,Y(\vartheta,\varphi)$$

$$Y(\vartheta,\varphi)\cdot\frac{1}{r}\frac{d^2}{dr^2}(rR(r)) + \frac{2m}{\hbar^2}(E-U(r))R(r)Y(\vartheta,\varphi) + \frac{1}{r^2}R(r)\Lambda Y(\vartheta,\varphi) = 0 \;/\cdot\frac{R\,Y}{r^2}$$

$$r^2\cdot\underbrace{\frac{\frac{1}{r}\frac{d^2}{dr^2}(rR_n) + \frac{2m}{\hbar^2}(E-U(r))R(r)}{R(r)}}_{-\lambda} + \underbrace{\frac{\Lambda Y(\vartheta,\varphi)}{Y}}_{\lambda} = 0$$

(ϑ,φ) - nezav. varijable

$\Rightarrow \Sigma\ -\lambda+\lambda = 0$

↓ treba odvojiti!

$$\frac{1}{Y}\cdot\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial Y}{\partial\vartheta}\right) + \frac{1}{Y}\cdot\frac{1}{\sin^2\vartheta}\frac{\partial^2 Y}{\partial\varphi^2} = \lambda \qquad Y(\vartheta,\varphi) = \Theta(\vartheta)\,\phi(\varphi)$$

i) $\Lambda Y = \lambda\cdot Y$ ← problem svojstv. vrij. i fja. (kao u poč. Schröd.)

ii) $\frac{1}{r}\frac{d^2}{dr^2}(rR) + \left[\frac{2m}{\hbar^2}(E-U(r)) + \frac{\lambda}{r^2}\right]R(r) = 0$

→ uvjeti na λ iz regularnosti rješ. za $\forall$ $0\le\varphi\le 2\pi$, $0\le\vartheta\le\pi$

$Y(\vartheta,\varphi)$ - konačna, neprek., jednozn. fja.

..... prorad: !!! - Matem. dopuna - Supek I 585. & 82.

$\Rightarrow$ (21a) $\lambda = -l(l+1)$ $l = 0,1,2,\dots$ jer za $l\notin\mathbb{Z}$ dobili bi Legendr. fju. pa ne polinom

nalaze $m\in\mathbb{Z}$ zbog jednoznačnosti a kasnije $m = \pm l, \pm(l-1), \dots 0$

jer $Y(\vartheta,\varphi) = \Theta(\vartheta)\phi(\varphi)$

$\Rightarrow \phi(\varphi) = Ae^{im\varphi} + Be^{-im\varphi}$ $m\in\mathbb{N}$

ili $= e^{\pm im\varphi}$ $m\in\mathbb{Z}$

iii) $$Y_l^m(\vartheta,\varphi) = \sqrt{\frac{2l+1}{4\pi}\frac{(l-|m|)!}{(l+|m|)!}}\,\underbrace{P_l^m(\cos\vartheta)}_{\text{pridruž. Legendr. polinom}}\,e^{im\varphi}$$

gdje je ta kuglina fja. normirana na kuglu (jedinicu)

$$\int_0^{2\pi}\int_0^{\pi} Y_l^{m*}\cdot Y_{l'}^{m'}\,d\varphi\,\sin\vartheta\,d\vartheta = \delta_{mm'}\cdot\delta_{ll'}$$

$d\varphi$ $\sin\vartheta\,d\vartheta$ $= d\Omega$

→ proradi !!!

(31) a)

i) $\Lambda\, Y(\vartheta,\varphi) = \lambda \cdot Y(\vartheta,\varphi)$ $\quad \underline{\lambda \in R}$

Konstanta separacije problema

$\Lambda = \frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial}{\partial\vartheta}\right) + \frac{1}{\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}$

$\mu(r,\vartheta,\varphi) = R(r)\, Y(\vartheta,\varphi)$

$$\left[\frac{1}{\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2} + \frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial}{\partial\vartheta}\right) - \lambda\right] Y(\vartheta,\varphi) = 0$$

→ uvjeti regularnosti na valnu fju. ⇒

odabrati demo samo ona rješ. jbe., koja su konačna, napr. i jednoznačna za sve vrijednosti argumenta

$0 \le \varphi \le 2\pi \qquad 0 \le \vartheta \le \pi$

⇒ tim uvjetom ograničen je broj mogućih vrijednosti za $\underline{\lambda}$

$Y(\vartheta,\varphi) = \Theta(\vartheta)\,\phi(\varphi)$

$$\frac{\Theta}{\sin^2\vartheta}\frac{d^2\phi}{d\varphi^2} + \frac{\phi}{\sin\vartheta}\frac{d}{d\vartheta}\left(\sin\vartheta\frac{d\Theta}{d\vartheta}\right) - \lambda\,\Theta\phi = 0 \qquad / : \frac{\Theta\phi}{\sin^2\vartheta}$$

$$-\frac{1}{\phi}\frac{d^2\phi}{d\varphi^2} = +\left[\frac{\sin\vartheta}{\Theta}\frac{d}{d\vartheta}\left(\sin\vartheta\frac{d\Theta}{d\vartheta}\right) - \lambda\sin^2\vartheta\right] = K$$

$$\frac{d^2\phi}{d\varphi^2} + K\phi = 0$$

ii) $$\left[\frac{1}{\sin\vartheta}\frac{d}{d\vartheta}\left(\sin\vartheta\frac{d}{d\vartheta}\right) - \left(\lambda + \frac{K}{\sin^2\vartheta}\right)\right]\Theta = 0$$ (Θ)

$\phi(\varphi) = e^{\pm i\sqrt{K}\varphi}$

$e^{\pm i\sqrt{K}\varphi} = e^{\pm i\sqrt{K}(\varphi+2\pi)}$ jednoznačnost ⇒ $\underline{\sqrt{K} = m \in \mathbb{Z}}$ (m∈Z)

↑ periodičnost fja.

ii)' $t = \cos\vartheta \qquad \frac{d}{d\vartheta} = \frac{dt}{d\vartheta}\frac{d}{dt} = -\sin\vartheta\frac{d}{dt}$ $\quad \Rightarrow \underline{\phi(\varphi) = e^{im\varphi}}$

$\Theta(\vartheta) = \Theta(\arccos t) = \Theta_1(t)$ (Θ)

$$\left[\frac{1}{\sin\vartheta}(-\sin\vartheta)\frac{d}{dt}\cdot\left(\sin\vartheta\cdot(-\sin\vartheta)\frac{d}{dt}\right) - \left(\lambda + \frac{K}{\sin^2\vartheta}\right)\right]\Theta_1^{(t)} = 0$$

$$\left\{\frac{d}{dt}\left[(1-t^2)\frac{d}{dt}\right] - \left(\lambda + \frac{m^2}{1-t^2}\right)\right\}\Theta_1(t) = 0$$

Supek II

605. str.

$0 \le \vartheta \le \pi$

$t = \cos\vartheta \qquad 1 \ge t \ge -1$

$$\left\{ \underbrace{\frac{d}{dt}\left[(1-t^2)\frac{d}{dt}\right]}_{(1)} - \underbrace{\left(\lambda + \frac{m^2}{1-t^2}\right)}_{(2)} \right\} \Theta_1(t) = 0 \qquad (i)$$

$\Theta(\vartheta) = \sin^{-m}\vartheta \; S_\ell^{(m)}(\cos\vartheta)$

$\Theta_1(t) = (1-t^2)^{-\frac{m}{2}} \cdot S_\ell^m(t)$

bez motivacije za zadaću ?

- papir *) asimptotsko ponašanje $t^2 \to 1$ $\quad \vartheta \to 0, \pi$

$$(1) = (1-t^2)^{-\frac{m}{2}+1}\frac{d^2}{dt^2}S_\ell^m + 2(m-1)t(1-t^2)^{-\frac{m}{2}}\frac{d}{dt}S_\ell^m + \left[m(1-t^2)^{-\frac{m}{2}} + m^2t^2(1-t^2)^{-\frac{m}{2}-1}\right]S_\ell^m$$

$$(2) = \left[\lambda(1-t^2)^{-\frac{m}{2}} + m^2(1-t^2)^{-\frac{m}{2}-1}\right]S_\ell^m$$

$/\,(1-t^2)^{\frac{m}{2}}$

$$\Rightarrow (*)\quad (1-t^2)\frac{d^2}{dt^2}S_\ell^m(t) + 2(m-1)t\frac{d}{dt}S_\ell^m(t) + \left[-m(m-1) - \lambda\right]S_\ell^m(t) = 0$$

$$S_\ell^m(t) = \sum_{K=0}^{\infty} a_K t^K$$

$$(1-t^2)\sum_{K=2}^{\infty} a_K K(K-1)t^{K-2} + 2(m-1)t\sum_{K=1}^{\infty} a_K \cdot K t^{K-1} + \left[-\lambda - m(m-1)\right]\sum_{K=0}^{\infty} a_K t^K = 0$$

$$\sum_{K=2}^{\infty} a_K K(K-1)t^{K-2} - \sum_{K=2}^{\infty} a_K K(K-1)t^K + \sum_{K=1}^{\infty} 2(m-1)a_K \cdot K t^K + \left[-\lambda - m(m-1)\right]\sum_{K=0}^{\infty} a_K t^K = 0$$

$K-2 = K'$

$$\sum_{K=0}^{\infty} a_{K+2}(K+2)(K+1)t^K + \sum_{K=2}^{\infty}\left[-a_K K(K-1) + 2(m-1)a_K \cdot K + \left[-\lambda - m(m-1)\right]a_K\right]t^K +$$

$$+ 2(m-1)a_1 t + \left[-\lambda - m(m-1)\right]a_0 + \left[-\lambda - m(m-1)\right]a_1 t = 0$$

$$(K+2)(K+1)a_{K+2} + \left[-\lambda - K(K-1) + 2(m-1)K - m(m-1)\right]$$

$K=0 \qquad 2a_2 + \left[-\lambda - m(m-1)\right]a_0 = 0$

$K=1 \qquad 6a_3 + \left[-\lambda - (m-1)(m-2)\right]a_1 = 0$

(ii)

$$(K) \qquad (K+2)(K+1)a_{K+2} + \left[-\lambda - (m-K)(m-K-1)\right]a_K = 0$$

Supek II 586.

(str.) Koeficijenti parnih potencija odredeni su sa a_0, a koef. neparnih potencija sa a_1. Sami koeficijenti a_0 i a_1 ostaju neodredeni, i među njima nema veze. Prema tome, dobivamo dva linearno nezavisna rješenja s integracionim konstantama a_0 i a_1, od kojih jedno sadrži članove s parnim, a drugo s neparnim K.

*) $$\frac{a_{K+2}}{a_K} = \frac{\lambda + (m-K)(m-K-1)}{(K+2)(K+1)} \xrightarrow{K \gg |m|} 1$$

Kao geom. red. $1 + t^2 + t^4 + \ldots$ ili $t + t^3 + t^5 + \ldots = t(1 + t^2 + t^4 + \ldots)$

$\Rightarrow S_\ell^m(t)$ divergira za $|t| = 1$ ako $K \to \infty$

$t = \pm 1$

& $(1-t^2)^{-\frac{m}{2}}$ div. za $|t|=1$ ako $m \neq 0$

Supek II 585.

3. Legendreovi polinomi

fkt. izvodnica:

$$\phi(s,t) = \frac{1}{\sqrt{1-2st+s^2}} = \sum_{l=0}^{\infty} P_l(t)\, s^l \qquad |t| \le 1 \quad |s| < 1$$

konvergira daj ∞ reel

$$\frac{1}{1+(\pm s)} = \sum_{l=0}^{\infty} (\pm s)^l$$

→ $t = \pm 1$ $\quad \phi(s,\pm 1) = \frac{1}{1 \mp s} = \sum_{l=0}^{\infty} P_l(\pm 1)\, s^l$

$$= \sum_{l=0}^{\infty} (\pm 1)^l s^l$$

$$\Rightarrow \quad P_l(1) = 1 \qquad P_l(-1) = (-1)^l$$

$$\frac{\partial \phi}{\partial t} = -\frac{1}{2}(1-2st+s^2)^{-\frac{3}{2}}(-2s) = s(1-2st+s^2)^{-\frac{3}{2}} \qquad \frac{\partial \phi}{\partial s} = -\frac{1}{2}(1-2st+s^2)^{-\frac{3}{2}}(-2t+2s) = (t-s)(1-2st+s^2)^{-3/2}$$

$$\frac{\partial \phi}{\partial t} = \frac{s}{t-s}\frac{\partial \phi}{\partial s} \qquad \frac{\partial \phi}{\partial s} = \frac{t-s}{1-2st+s^2}\cdot \phi$$

$$\sum_{l=0}^{\infty} P_l'(t)\, s^l = \frac{s}{t-s}\sum_{l=1}^{\infty} l\, P_l(t)\, s^{l-1} \qquad \sum_{l=1}^{\infty} l\, P_l(t)\, s^{l-1} = \frac{t-s}{1-2st+s^2}\cdot \sum_{l=0}^{\infty} P_l(t)\, s^l$$

$$\sum_{l=0}^{\infty} t\, P_l'(t)\, s^l - \sum_{l=0}^{\infty} P_l'(t)\, s^{l+1} = \sum_{l=1}^{\infty} l\, P_l(t)\, s^l \qquad \sum_{l=1}^{\infty} l\, P_l(t)\, s^{l-1} - \sum_{l=1}^{\infty} 2lt\, P_l(t)\, s^l + \sum_{l=1}^{\infty} l\, P_l(t)\, s^{l+1} = \sum_{l=0}^{\infty} t\, P_l(t)\, s^l - \sum_{l=0}^{\infty} P_l(t)\, s^{l+1}$$

$$\sum_{l=0}^{\infty} t\, P_l'(t)\, s^l - \sum_{l=1}^{\infty} P_{l-1}'(t)\, s^l = \sum_{l=1}^{\infty} l\, P_l(t)\, s^l \qquad \sum_{l=0}^{\infty} (l+1) P_{l+1}(t)\, s^l - \sum_{l=1}^{\infty} 2lt\, P_l(t)\, s^l + \sum_{l=2}^{\infty} (l-1) P_{l-1}(t)\, s^l = \sum_{l=0}^{\infty} t\, P_l(t)\, s^l - \sum_{l=1}^{\infty} P_{l-1}(t)\, s^l$$

množe $l=0$ množe $l=1$ ipr $l+1=0$

$t \cdot P_0'(t) = 0$ za $l=0$ $\qquad P_1(t) - t\, P_0(t) = 0$ za $l=0$

za $l=1,2,\ldots$

$$t\, P_l'(t) - P_{l-1}'(t) - l\, P_l(t) = 0 \qquad (l+1) P_{l+1}(t) - (2l+1)\, t\, P_l(t) + l\, P_{l-1}(t) = 0$$

$l = 0,1,2,\ldots$ $\quad P_{-1}'(t) = 0$ za $l = 0,1,2,\ldots$ $\quad P_{-1}(t) \equiv 0$

$$\Rightarrow \quad P_{l-1}' = t\, P_l' - l\, P_l \qquad (l+1) P_{l+1}' - (2l+1) P_l - (2l+1) t\, P_l' + l\, P_{l-1}' = 0$$

$$(l+1) P_{l+1}' - (l^2+2l+1) P_l - (l+1) t\, P_l' = 0 \qquad +lt\, P_l' - l^2 P_l$$

$$\Rightarrow \quad P_{l+1}' - (l+1) P_l - t\, P_l' = 0 \quad (*)$$

ili $l+1 \to l$

$$P_l' - l\, P_{l-1} - t\, P_{l-1}' = 0 \quad \to \quad P_l' - l\, P_{l-1} - t^2 P_l' + lt\, P_l = 0$$

$$(1-t^2) P_l' - l\, P_{l-1} + lt\, P_l = 0 \qquad \Big/\frac{d}{dt} \to (1-t^2) P_l'' - 2t\, P_l' + l\, P_l + lt\, P_l' - l(t P_l' - l P_l) = 0$$

$$\Rightarrow \quad \left[(1-t^2)\frac{d^2}{dt^2} - 2t\frac{d}{dt} + l(l+1)\right] P_l(t) = 0 \quad *)$$

$$P_l(t) = \sum_{K=0}^{\infty} a_K t^K$$

$$\Rightarrow \quad a_{K+2} = a_K \frac{K(K+1) - l(l+1)}{(K+2)(K+1)}$$

kao (*) za $m=0$ & $\lambda = -l(l+1)$

a_0 & a_1 određuju dva lin. nezav. rješenja

- ako λ proizv. konst. oba reda beskonačna i konvergiraju za $|t|<1$, a divergiraju za $|t|=1$ *)
- ako $\lambda = -l(l+1)$ $l \in Z$ tada se jedan od redova potencija prekida s članom $K = \begin{Bmatrix} l \\ -l-1 \end{Bmatrix}$ $K = l$ jer $K = \begin{Bmatrix} m+l \\ m-l-1 \end{Bmatrix}_{m=0}$

→ jedno rješenje jbe. *) je beskonačan red, koji divergira za $|t|=1$ ↓ fizički neinteresantno

drugo, regularno rješenje je polinom l-tog stupnja, to je Legendre-ov polinom $P_l(t)$

1° $l \in Z$ $l \geq 0$ & $K \geq 0$ $\Rightarrow K = l$ prekid parnog ili neparnog reda potencija ovisno da li je l paran ili neparan

2° $l_1 \in Z$ $l_1 < 0$ & $K \geq 0$ $\Rightarrow K = -l_1 - 1$ prekid parnog ili neparnog reda potencija ovisno da li je l neparan ili paran

↑ nepotrebno jer ∃ korespodencija:

$l \geq 0$	0	1	2	3	4	}
	↕	↕	↕	↕	↕	
$l_1 < 0$	-1	-2	-3	-4	-5	

$\Rightarrow \underline{l_1 = -l-1}$ $\quad \underline{\lambda = -l_1(l_1+1) = -(-l-1)[(-l-1)+1] = -l(l+1)}$

$l = -l_1 - 1$ $\quad K = -l_1 - 1 = l$

tj. ako $l \in \{-N\}$ ne dobivamo ništa novo, već iste polinome kao kad $l \in \{0\} \cup \{N\}$

→ potražimo lin. dif. jbu. 1. reda za fju.

$$y(t) = (t^2-1)^l$$

$$y'(t) = l(t^2-1)^{l-1} \cdot 2t = \frac{2lt}{t^2-1}(t^2-1)^l$$

$$(t^2-1)y' - 2lty = 0 \quad / \frac{d}{dt}$$

$$(t^2-1)y'' + 2ty' - 2lty' - 2ly = 0$$

$$(t^2-1)y'' - 2(l-1)ty' - 2ly = 0 \quad / \left(\frac{d}{dt}\right)^l$$

(31) c)

matem. ind:

$l=1 \quad (t^2-1)\frac{d}{dt}y'' + y''\cdot 2t$

$l=2 \quad (t^2-1)\frac{d^2}{dt^2}y'' + 4t\frac{d^2}{dt^2}y' + 2(2-1)\frac{d^2}{dt^2}y$

$l+1 \quad (t^2-1)\left(\frac{d}{dt}\right)^{l+1}y'' + 2t(l+1)\left(\frac{d}{dt}\right)^{l+1}y' + 2l\left(\frac{d}{dt}\right)^{l+1}y + l(l-1)\left(\frac{d}{dt}\right)^{l+1}y$

$(l+1)\,l$

$\left(\frac{d}{dt}\right)^{l-2}\left(\frac{d}{dt}\right)^2 \qquad (t^2-1)\frac{d}{dt}y'' + y''\cdot 2t$

$(t^2-1)\frac{d^2}{dt^2}y'' + 2t\frac{d}{dt}y'' + 2t\frac{d}{dt}y'' + 2\frac{d^2}{dt^2}y$

$$\left(\frac{d}{dt}\right)^l\left[y''(t^2-1)\right] = (t^2-1)\left(\frac{d}{dt}\right)^l y'' + 2tl\left(\frac{d}{dt}\right)^l y' + l(l-1)\left(\frac{d}{dt}\right)^l y$$

$$\left(\frac{d}{dt}\right)^l(y't) = t\left(\frac{d}{dt}\right)^l y' + l\left(\frac{d}{dt}\right)^l y \qquad l+1 \qquad t\left(\frac{d}{dt}\right)^{l+1}y' + \left(\frac{d}{dt}\right)^{l+1}y + l\left(\frac{d}{dt}\right)^{l+1}y \quad (l+1)$$

$$(t^2-1)\frac{d^2}{dt^2}\left(\frac{d}{dt}\right)^l y + 2tl\frac{d}{dt}\left(\frac{d}{dt}\right)^l y + l(l-1)\left(\frac{d}{dt}\right)^l y$$
$$-2(l-1)t\frac{d}{dt}\left(\frac{d}{dt}\right)^l y - 2(l-1)l\left(\frac{d}{dt}\right)^l y - 2l\left(\frac{d}{dt}\right)^l y = 0$$

$-l(l-1)+l = -l^2+l-2l = -l^2-l$

$$\left[(t^2-1)\frac{d^2}{dt^2} + 2t\frac{d}{dt} - l(l+1)\right]\left(\frac{d}{dt}\right)^l y = 0$$

$\binom{l}{0} = \binom{l+1}{0}\binom{l}{l} + \binom{l+1}{l+1}$

$$\left[(1-t^2)\frac{d^2}{dt^2} - 2t\frac{d}{dt} + l(l+1)\right]\left(\frac{d}{dt}\right)^l y = 0 \quad \Leftrightarrow \; *)$$

$r = 1, \dots, l$

$\binom{l}{r-1} + \binom{l}{r} = \binom{l+1}{r}$

$\frac{l(l-1)\cdots(l-r+1)}{r!} + \frac{l\cdots(l-r+1)}{r!} = \frac{(l+1)\cdots(l-r+2)}{r!}$

$= \frac{l(l-1)\cdots(l-r+2)\,[r+l-r+1]}{r!}$

$\Rightarrow$ budući je $\left(\frac{d}{dt}\right)^l y$ polinom, a drugo množ. je st. reda

$l=1 \quad (u\cdot v)' = \binom{1}{0}u'v + \binom{1}{1}uv'$

$$(u\cdot v)^{(l+1)} = \sum_{r=0}^{l}\binom{l}{r}\left[u^{(r+1)}v^{(l-r)} + u^{(r)}v^{(l-r+1)}\right] = \sum_{r=0}^{l}\binom{l}{r}u^{(r+1)}v^{(l-r)} + \sum_{r=0}^{l}u^{(r)}v^{(l+1-r)}$$

$$= \sum_{r=0}^{l+1}\binom{l+1}{r}u^{(r)}v^{(l+1-r)}$$

$$(u\cdot v)^{(l)} = \sum_{r=0}^{l}\binom{l}{r}u^{(r)}\cdot v^{(l-r)}$$

$$\Rightarrow \quad \underline{\left(\frac{d}{dt}\right)^l(t^2-1)^l = C_l\,P_l(t)}$$

$C_l = (-1)^l\left[\;\right]_{t=-1} = (-1)^l\cdot l!\,(-2)^l$

$$\underline{P_l(1)=1} \quad \Rightarrow \quad C_l = \left[\left(\frac{d}{dt}\right)^l(t^2-1)^l\right]_{t=1}$$

$$= \left[\sum_{r=0}^{l}\binom{l}{r}\cdot l(l-1)\cdots(l-r+1)\cdot l(l-1)\cdots(r+1)\,(t+1)^{l-r}\cdot(t-1)^r\right]_{t=1}$$

$(t+1)^l(t-1)^l$

$$= \left[\binom{l}{0}\cdot l(l-1)\cdots 1\cdot(t+1)^l\right]_{t=1} = l!\,2^l$$

$$\Rightarrow \quad \underline{C_l = l!\,2^l}$$

$$\underline{P_l(t) = \frac{1}{2^l\cdot l!}\left(\frac{d}{dt}\right)^l(t^2-1)^l}$$

Rodrigues-ova formula za Legandreov polinom - polinom l-tog stupnja

$l+K \qquad K>l$

$$\int_{-1}^{+1}P_l(t)P_K(t)\,dt = \frac{1}{2^l\cdot l!\,2^K\cdot K!}\int_{-1}^{1}\left[\left(\frac{d}{dt}\right)^l(t^2-1)^l\right]\left[\left(\frac{d}{dt}\right)^K(t^2-1)^K\right]dt =$$

$\mu \qquad dV$

$$= \frac{1}{2^{l+K}\cdot l!\,K!}\left\{\left[\left(\frac{d}{dt}\right)^l(t^2-1)^l\right]\left[\left(\frac{d}{dt}\right)^{K-1}(t^2-1)^K\right] - \int\left[\left(\frac{d}{dt}\right)^{l+1}(t^2-1)^l\right]\left[\left(\frac{d}{dt}\right)^{K-1}(t^2-1)^K\right]dt\right\}_{-1}^{1} =$$

$$\left\{\left(\frac{d}{dt}\right)^{K-1}(t^2-1)^K\right\}_{-1}^{1} = \left\{\sum_{r=0}^{K-1}\binom{K-1}{r}k(k-1)\cdots(k-r+1)\;k(k-1)\cdots(r+2)\,(t+1)^{K-r}(t-1)^{r+1}\right\}_{-1}^{1} = 0-0=0$$

$k(k-1)\cdots(r+2) = \frac{k!}{(r+1)!}$

$1 \le s \le K$

$$\left(\frac{d}{dt}\right)^{K-s}(t^2-1)^K = \sum_{n=0}^{K-s}\binom{K-s}{n} K(K-1)\cdots(K-n+1)\,K(K-1)\cdots(n+s+1)\,(t+1)^{K-n}(t-1)^{n+s} \Big|_{-1}^{1} = 0 - 0 = 0$$

$K-(K-s-n)$

$$= -\frac{1}{2^{l+K}\cdot l!\,K!}\int_{-1}^{1}\left[\left(\frac{d}{dt}\right)^{l+1}(t^2-1)^l\right]\left[\left(\frac{d}{dt}\right)^{K-1}(t^2-1)^K\right]dt$$

$$= \frac{(-1)^K}{2^{l+K}\,l!\,K!}\int_{-1}^{1}(t^2-1)^K\left(\frac{d}{dt}\right)^{l+K}(t^2-1)^l\,dt$$

$K > l \Rightarrow l+K > 2l \Rightarrow \left(\frac{d}{dt}\right)^{l+K}(t^2-1)^l = 0$

$$\Rightarrow \int_{-1}^{1} P_l(t)\,P_k(t)\,dt = 0 \quad \text{za } \underline{l \neq K}$$

→ napomena!
za $l > K$ postupak bi išao po l

$\to \left(\frac{d}{dt}\right)^{K+l}(t^2-1)^K = 0$

$l > K \Rightarrow K+l > 2K$

$n-l \ge 0$? $\quad l-n \ge 0 \Rightarrow n-l \le 0$ $\Big\}$ $n-l=0$

$\underline{K=l}$ $\quad \left(\frac{d}{dt}\right)^{2l}(t^2-1)^l = (2l)!$

$$\sum_{n=0}^{2l}\binom{2l}{n} l(l-1)\cdots(l-n+1)\,l(l-1)\cdots(l-(2l-n)+1)\,(t+1)^{l-n}(t-1)^{n-l} = \binom{2l}{l} l!\,l! = \frac{(2l)\cdots(2l-l+1)\cdot l!}{l!}\,l! = (2l)!$$

$$\Rightarrow \int_{-1}^{1}\left[P_l(t)\right]^2 dt = \frac{(-1)^l\cdot(2l)!}{2^{2l}\cdot(l!)^2}\int_{-1}^{1}\left[(t+1)(t-1)\right]^l dt$$

$$\int_{-1}^{1}(t+1)^l(t-1)^l dt = \left[(t+1)^l\frac{1}{l+1}(t-1)^{l+1}\right]_{-1}^{1} - \frac{l}{l+1}\int_{-1}^{1}(t+1)^{l-1}(t-1)^{l+1}dt = \frac{(-1)^l\,l!}{(l+1)(l+2)\cdots(2l)}\int_{-1}^{1}(t-1)^{2l}dt$$

$$= \frac{(-1)^l\cdot(l!)^2\cdot 2^{2l+1}}{(2l)!\,(2l)}$$

$$\frac{1}{2l+1}(t-1)^{2l+1}\Big]_{-1}^{1} = -\frac{1}{2l+1}(-2)^{2l+1} = \frac{1}{2l+1}2^{2l+1}$$

$$\int_{-1}^{1}\left[P_l(t)\right]^2 dt = \frac{(-1)^l}{2^{2l}}\frac{(2l)!}{(l!)^2}\cdot\frac{(-1)^l(l!)^2\,2\cdot 2^{2l}}{(2l)!\,(2l+1)} = \frac{2}{2l+1}$$

$$\Rightarrow \int_{-1}^{1} P_l(t)\,P_k(t)\,dt = \frac{2}{2l+1}\,\delta_{kl}$$

Uvedimo fje:

$$X_l(t) = \sqrt{\frac{2l+1}{2}}\,P_l(t)$$

$$\Rightarrow \int_{-1}^{1} X_l(t)\,X_k(t)\,dt = \delta_{kl}$$

→ jbu. *) deriviramo $|m|$ puta po t

$$\left[(1-t^2)\frac{d^2}{dt^2} - 2t\frac{d}{dt} + \underbrace{l(l+1)}_{(-\lambda)}\right] P_l(t) = 0 \quad / \left(\frac{d}{dt}\right)^{|m|}$$

sa (31 c) =>

$$\left\{(1-t^2)\left(\frac{d}{dt}\right)^{|m|+2} - 2t\,|m|\left(\frac{d}{dt}\right)^{|m|+1} - |m|(|m|-1)\left(\frac{d}{dt}\right)^{|m|} - 2t\left(\frac{d}{dt}\right)^{|m|+1} - 2|m|\left(\frac{d}{dt}\right)^{|m|} + l(l+1)\left(\frac{d}{dt}\right)^{|m|}\right\} P_l(t) = 0$$

(i)
$$\left\{(1-t^2)\left(\frac{d}{dt}\right)^{|m|+2} - 2t(|m|+1)\left(\frac{d}{dt}\right)^{|m|+1} + \left[\underbrace{l(l+1)}_{-\lambda} - |m|(|m|+1)\right]\left(\frac{d}{dt}\right)^{|m|}\right\} P_l(t) = 0$$

$(l-|m|)[l+|m|+1]$

→ **Definiramo** pridružene Legendre-ove polinome m-tog reda:

Def 1.
$$P_l^m(t) \overset{def.}{=} (1-t^2)^{\frac{|m|}{2}} \underbrace{\left(\frac{d}{dt}\right)^{|m|} P_l(t)}_{= S_*^{|m|} \text{ u MMF-u}} \qquad m = 0, \pm1, \pm2, \ldots \pm l$$

polinom $(l-|m|)$ stupnja

m -paran P_l^m polinom l-tog stupnja $(1-t^2)^{\frac{2s}{2}}$ $\quad 2s+(l-2s)=l$

m -neparan P_l^m polinom $(l-1)$ -vog stupnja pomnožen s $\sqrt{1-t^2}$

$(1-t^2)^{\frac{2s+1}{2}} = (1-t^2)^s \cdot \sqrt{1-t^2}$ $\quad 2s+(l-(2s+1)) = l-1$

$m=0$ $\quad P_l^0(t) = P_l(t)$

def. =>
$$P_l^m(t) = \frac{1}{2^l l!}(1-t^2)^{\frac{|m|}{2}}\left(\frac{d}{dt}\right)^{l+|m|}(t^2-1)^l$$

$l=0$ $\quad P_0^0 = 1$

$l=1$ $\quad P_1^0 = t \qquad P_1^1 = \sqrt{1-t^2}$

$l=2$ $\quad P_2^0 = \frac{1}{2}(3t^2-1) \qquad P_2^1 = 3t\sqrt{1-t^2} \qquad P_2^2 = 3(1-t^2)$

$l=3$ $\quad P_3^0 = \frac{t}{2}(5t^2-3) \qquad P_3^1 = \frac{3}{2}(5t^2-1)\sqrt{1-t^2} \qquad P_3^2 = 15t(1-t^2) \qquad P_3^3 = 15(1-t^2)^{3/2}$

$$\left(\frac{d}{dt}\right)^{|m|} P_l(t) = (1-t^2)^{-\frac{|m|}{2}} P_l^m(t)$$

$|m|(1-t^2)^{\frac{|m|}{2}-1} + |m|t\left(\frac{|m|}{2}+1\right)\frac{d}{dt}(1-t^2)^{\frac{|m|}{2}-2}$

$$\left(\frac{d}{dt}\right)^{|m|+1} P_l(t) = \left[(1-t^2)^{-\frac{|m|}{2}}\frac{d}{dt} + |m|t(1-t^2)^{-\frac{|m|}{2}-1}\right] P_l^m(t)$$

$$\left(\frac{d}{dt}\right)^{|m|+2} P_l(t) = \left[(1-t^2)^{-\frac{|m|}{2}}\frac{d^2}{dt^2} + 2|m|t(1-t^2)^{-\frac{|m|}{2}-1}\frac{d}{dt} + \left(\frac{|m|+2}{1-t^2}t^2+1\right)|m|(1-t^2)^{-\frac{|m|}{2}-1}\right] \cdot P_l^m(t)$$

→ uvrstimo u (i)

$$\left\{\left[(1-t^2)^{-\frac{|m|}{2}+1}\frac{d^2}{dt^2} + 2|m|t(1-t^2)^{-\frac{|m|}{2}}\frac{d}{dt} + \left(\frac{|m|+2}{1-t^2}t^2+1\right)|m|(1-t^2)^{-\frac{|m|}{2}}\right] + \left[-2(|m|+1)(1-t^2)^{-\frac{|m|}{2}}t\frac{d}{dt} - 2|m|(|m|+1)t^2(1-t^2)^{-\frac{|m|}{2}-1}\right]\right.$$

$$\left. + \left[l(l+1) - |m|(|m|+1)\right](1-t^2)^{-\frac{|m|}{2}}\right\} P_l^m(t) = 0 \quad / \cdot (1-t^2)^{\frac{|m|}{2}}$$

$|m|(|m|+2) - 2|m|(|m|+1) = |m|(|m|+2-2|m|-2) = -|m||m|$

$$\left\{ [(1-t^2)\frac{d^2}{dt^2} + 2|m|t\frac{d}{dt} + \left(\frac{|m|+2}{1-t^2}t^2+1\right)|m|] + [-2(|m|+1)t\frac{d}{dt} - 2|m|(|m|+1)t^2(1-t^2)^{-1}] + \right.$$
$$\left. + [l(l+1) - |m|(|m|+1)] \right\} P_l^m(t) = 0$$

$\frac{-m^2t^2}{1-t^2} - m^2 = -m^2\frac{t^2+1-t^2}{1-t^2}$

i) $$\left\{ (1-t^2)\left(\frac{d}{dt}\right)^2 - 2t\frac{d}{dt} + \left[l(l+1) - \frac{m^2}{1-t^2}\right] \right\} P_l^m(t) = 0$$

dif. jba. pridruženih Legendreovih polinoma

(31) b) $\Rightarrow$ $t P_l'(t) - P_{l-1}'(t) - l P_l(t) = 0 \quad / \left(\frac{d}{dt}\right)^{|m|-1}$ $\qquad (l+1)P_{l+1}(t) - (2l+1)tP_l(t) + lP_{l-1}(t) = 0 \quad / \left(\frac{d}{dt}\right)^{|m|}$ (*)

$t\left(\frac{d}{dt}\right)^{|m|}P_l(t) + (|m|-1)\left(\frac{d}{dt}\right)^{|m|}P_l(t) - \left(\frac{d}{dt}\right)^{|m|}P_{l-1}(t) - l\left(\frac{d}{dt}\right)^{|m|+1}P_l(t) = 0 \qquad (l+1)\left(\frac{d}{dt}\right)^{|m|}P_{l+1} - (2l+1)\left[t\left(\frac{d}{dt}\right)^{|m|}P_l + |m|\left(\frac{d}{dt}\right)^{|m|-1}P_l\right] + l\left(\frac{d}{dt}\right)^{|m|}P_{l-1} = 0$

(1) $t\left(\frac{d}{dt}\right)^{|m|}P_l + (|m|-l-1)\left(\frac{d}{dt}\right)^{|m|-1}P_l - \left(\frac{d}{dt}\right)^{|m|}P_{l-1} = 0 \quad / \cdot |m|$ (2) $(l+1)\left(\frac{d}{dt}\right)^{|m|}P_{l+1} - (2l+1)t\left(\frac{d}{dt}\right)^{|m|}P_l - (2l+1)|m|\left(\frac{d}{dt}\right)^{|m|-1}P_l + l\left(\frac{d}{dt}\right)^{|m|}P_{l-1} = 0$

(31) b (*) $\Rightarrow$ $P_{l+1}' - (l+1)P_l - tP_l' = 0 \quad / \left(\frac{d}{dt}\right)^{|m|-1}$

(3) $\left(\frac{d}{dt}\right)^{|m|}P_{l+1} - (l+|m|)\left(\frac{d}{dt}\right)^{|m|-1}P_l - t\left(\frac{d}{dt}\right)^{|m|}P_l = 0$

(1) + (3) $\Rightarrow$ $\left(\frac{d}{dt}\right)^{|m|}P_{l+1} - (2l+1)\left(\frac{d}{dt}\right)^{|m|-1}P_l - \left(\frac{d}{dt}\right)^{|m|}P_{l-1} = 0 \quad / (-|m|)$

(4) $-|m|\left(\frac{d}{dt}\right)^{|m|}P_{l+1} + (2l+1)|m|\left(\frac{d}{dt}\right)^{|m|-1}P_l + |m|\left(\frac{d}{dt}\right)^{|m|}P_{l-1} = 0 \quad / \cdot (1-t^2)^{\frac{|m|}{2}}$

(2) + (4) $\Rightarrow$ $$(l-|m|+1)P_{l+1}^m - (2l+1)tP_l^m + (l+|m|)P_{l-1}^m = 0$$

rekurzivna relacija istih, gornjih indeksa

(31) b) $\Rightarrow$ $tP_l' - P_{l-1}' - lP_l = 0 \qquad (l+1)P_{l+1}' - (2l+1)P_l - (2l+1)tP_l' + lP_{l-1}' = 0$

$\Rightarrow$ $P_{l+1}' - P_{l-1}' - (2l+1)P_l = 0 \quad / \left(\frac{d}{dt}\right)^{|m|}$

$\left(\frac{d}{dt}\right)^{|m|+1}P_{l+1} - \left(\frac{d}{dt}\right)^{|m|+1}P_{l-1} = (2l+1)\left(\frac{d}{dt}\right)^{|m|}P_l \quad / (1-t^2)^{\frac{|m|+1}{2}}$

$$P_{l+1}^{m+1} - P_{l-1}^{m+1} = (2l+1)\sqrt{1-t^2}\,P_l^m$$

$$\left\{ \frac{d}{dt}\left[(1-t^2)\frac{d}{dt}\right] + \left[l(l+1) - \frac{m^2}{1-t^2}\right] \right\} P_l^m(t) = 0 \quad / \cdot P_{l'}^{m'}(t)$$

$$\left\{ \frac{d}{dt}\left[(1-t^2)\frac{d}{dt}\right] + \left[l'(l'+1) - \frac{m'^2}{1-t^2}\right] \right\} P_{l'}^{m'}(t) = 0 \quad / \cdot P_l^m(t)$$

$P_{l'}^{m'}\frac{d}{dt}\left[(1-t^2)\frac{dP_l^m}{dt}\right] - P_l^m\frac{d}{dt}\left[(1-t^2)\frac{dP_{l'}^{m'}}{dt}\right] + (m'^2-m^2)\frac{P_{l'}^{m'}P_l^m}{1-t^2} + [l(l+1) - l'(l'+1)]P_{l'}^{m'}P_l^m = 0 \quad \Big/ \int_{-1}^{1}$

$\frac{d}{dt}\left[(1-t^2)\left(P_{l'}^{m'}\frac{dP_l^m}{dt} - P_l^m\frac{dP_{l'}^{m'}}{dt}\right)\right] = P_{l'}^{m'}\frac{d}{dt}\left[(1-t^2)\frac{dP_l^m}{dt}\right] - P_l^m\frac{d}{dt}\left[(1-t^2)\frac{dP_{l'}^{m'}}{dt}\right] + (1-t^2)\frac{dP_l^m}{dt}\cdot\frac{dP_{l'}^{m'}}{dt} + (1-t^2)\frac{dP_{l'}^{m'}}{dt}\cdot\frac{dP_l^m}{dt}$

$$\left[(1-t^2)\left(P_{l'}^{m'}\frac{d}{dt}P_l^m - P_l^m\frac{d}{dt}P_{l'}^{m'}\right)\right]_{-1}^{1} + (m'^2-m^2)\int_{-1}^{1}\frac{P_{l'}^{m'}P_l^m}{1-t^2}dt + [l(l+1) - l'(l'+1)]\int_{-1}^{1}P_{l'}^{m'}P_l^m dt = 0$$

(31) e)

$(l-l')[l+l'+1]$

$l^2+l \quad -l'^2-l'$

$$[l(l+1)-l'(l'+1)]\int_{-1}^{1} P_{l'}^{m'} P_l^m \, dt = (m^2-m'^2)\int_{-1}^{1} \frac{P_{l'}^{m'} P_l^m}{1-t^2}\, dt \qquad (ii')$$

$\frac{1}{1-t^2}$ - težinski faktor

$l=l' \quad m \neq m' \Rightarrow \int_{-1}^{1} \frac{P_{l'}^{m'} P_l^m}{1-t^2}\, dt = 0$

inače $m^2 \neq m'^2$ kad

def. $P_l^m = (1-t^2)^{\frac{m}{2}} \left(\frac{d}{dt}\right)^m P_l$ $m \in \mathbb{N}$

$l \neq l' \quad m = m' \Rightarrow \int_{-1}^{1} P_{l'}^{m'} P_l^m \, dt = 0$

① $l \neq l' \quad m \neq m'$ vrijedi (ii')

$l = l' \quad m = m' \Rightarrow$

$$\int_{-1}^{1} [P_l^m(t)]^2 dt = \int_{-1}^{1} (1-t^2)^{|m|} \left[\left(\frac{d}{dt}\right)^{|m|} P_l(t)\right]^2 dt$$

$u = (1-t^2)^{|m|}\left(\frac{d}{dt}\right)^{|m|} P_l(t)$

$dv = \left(\frac{d}{dt}\right)^{|m|} P_l(t)\, dt$

$$= \left[(1-t^2)^{|m|}\left(\frac{d}{dt}\right)^{|m|} P_l(t)\left(\frac{d}{dt}\right)^{|m|-1} P_l(t)\right]_{-1}^{1} - \int_{-1}^{1} \left(\frac{d}{dt}\right)^{|m|-1} P_l \frac{d}{dt}\left[(1-t^2)^{|m|}\left(\frac{d}{dt}\right)^{|m|} P_l\right] dt$$

$$= -\int_{-1}^{1} \left[\left(\frac{d}{dt}\right)^{|m|-1} P_l\right] \frac{d}{dt}\left[(1-t^2)^{|m|}\left(\frac{d}{dt}\right)^{|m|} P_l\right] dt$$

② d)

(i) $|m| \to |m|-1$ $\left\{(1-t^2)\left(\frac{d}{dt}\right)^{|m|+1} - 2t|m|\left(\frac{d}{dt}\right)^{|m|} + (l+|m|)(l-|m|+1)\left(\frac{d}{dt}\right)^{|m|-1}\right\} P_l(t) = 0 \quad / (1-t^2)^{|m|-1}$

$$\frac{d}{dt}\left[(1-t^2)^{|m|}\left(\frac{d}{dt}\right)^{|m|} P_l\right] = -(l+|m|)(l-|m|+1)(1-t^2)^{|m|-1}\left(\frac{d}{dt}\right)^{|m|-1} P_l$$

$$\Rightarrow \int_{-1}^{1} (P_l^m)^2 dt = (l+|m|)(l-|m|+1)\int_{-1}^{1} \left[\left(\frac{d}{dt}\right)^{|m|-1} P_l(t)\right]^2 (1-t^2)^{|m|-1} dt$$

$(1-t^2)^{\frac{|m|-1}{2}} \cdot (1-t^2)^{\frac{|m|-1}{2}}$

$$= (l+|m|)(l-|m|+1)\int_{-1}^{1} (P_l^{m-1})^2 dt$$

- postupak kojim snižavamo m-ove

$|m|=2 \quad |m|=1$

$$\int_{-1}^{1} (P_l^m)^2 dt = [(l+|m|)(l+|m|-1)\cdots(l+2)(l+1)] \cdot [(l-|m|+1)(l-|m|+2)\cdots(l-1)l] \int_{-1}^{1} (P_l^0)^2 dt$$

$|m|-1 \qquad 0=1-1$

$$= \frac{(l+|m|)!}{l!} \cdot \frac{l!}{(l-|m|)!} \cdot \frac{2}{2l+1}$$

$m = m'$

$$\int_{-1}^{1} P_{l'}^m(t) \cdot P_l^m(t) dt = \frac{(l+|m|)!}{(l-|m|)!} \cdot \frac{2}{2l+1} \delta_{ll'}$$

$l \neq l'$ $m \neq m'$ & (ii) $\Rightarrow$

$$\int_{-1}^{1} \frac{P_{l'}^{m'} P_l^m}{1-t^2}\,dt = \frac{(l-l')(l+l'+1)}{(|m|-|m'|)(|m|+|m'|)} \int_{-1}^{1} P_{l'}^{m'} P_l^m\,dt$$

napomena: (2) strogost gor se vrši o pliskontinuiranom linesu → strogo Mitrinović str. (37)

→ granični prijelaz $|m| \to |m'|$ & $l \to l'$

$$\Rightarrow \int_{-1}^{1} \frac{(P_l^m)^2}{1-t^2}\,dt = \frac{2l+1}{2|m|} \int_{-1}^{1} (P_l^m)^2\,dt = \frac{(l+|m|)!}{|m|(l-|m|)!}$$

$l = l'$

$$\int_{-1}^{1} \frac{P_l^{m'}(t) P_l^m(t)}{1-t^2}\,dt = \frac{(l+|m|)!}{|m|(l-|m|)!}\,\delta_{mm'}$$

$= S_*^{'m}(t)$ u MMF-u

Def 2. $P_l^m(t) \overset{def.}{=} (1-t^2)^{\frac{m}{2}} \left(\frac{d}{dt}\right)^m P_l(t)$

→ za $m<0$ dolazimo do polinoma s negativnim gornjim indeksom (i)

→ sve do sada izvedene relacije vrijede za $m \geq 0$, i razmatranje treba proširiti i za $m<0$

→ dif. jbu. i) (koju smo dobivali rješavajući problem $\Delta Y = \lambda Y$) zadovoljavaju i polinomi sa $m<0$, jer m ulazi kao kvadrat

def. $\Rightarrow$ $P_l^{-m}(t) = \frac{1}{2^l l!} (1-t^2)^{-\frac{m}{2}} \left(\frac{d}{dt}\right)^{l-m} (t^2-1)^l$ $\quad m \geq 0$

MMF $\overset{(*)}{\Rightarrow}$ Jacoby-ov identitet $\left(\frac{d}{dt}\right)^{l-m} (t^2-1)^l = \frac{(-1)^m (l-m)!}{(l+m)!} (1-t^2)^m \left(\frac{d}{dt}\right)^{l+m} (t^2-1)^l$

$l-m \geq 0 \Rightarrow m \leq l$, $l+m \geq 0 \Rightarrow m \geq -l$, za $|m| \leq l$

$P_l^{-m}(t) = \frac{1}{2^l l!} \frac{(-1)^m (l-m)!}{(l+m)!} (1-t^2)^{-\frac{m}{2}} \cdot (1-t^2)^m \left(\frac{d}{dt}\right)^{l+m} (t^2-1)^l = \frac{(-1)^m (l-m)!}{(l+m)!} \frac{1}{2^l l!} (1-t^2)^{\frac{m}{2}} \left(\frac{d}{dt}\right)^{l+m} (t^2-1)^l$

$$\Rightarrow P_l^{-m}(t) = (-1)^m \frac{(l-m)!}{(l+m)!} P_l^m(t) \quad \text{gdje } |m| \leq l$$

orig.

→ vidimo da je $P_l^{-m}(t)$ (*) regularno rješenje u cijelom području $-1 \leq t \leq 1$ (budući) je lin. zavisno od $P_l^m(t)$, što je u redu jer dif. jbn. i) ima samo jedno regularno rješenje, pa P_l^{-m} & P_l^m moraju biti lin. zavisni.

napomena!!! dakle, zbog fizičkog interesa dovoljno je da P_l^m definiramo sa **Def. 2.** jer su P_l^m & P_l^{-m} lin. zavisni, pa se broj rješenja ne povećava ako će $m<0$ uzimati P_l^{-m}, već faktora $e^{im\varphi}$ u $Y(\theta,\varphi)$

(31) f)

originalno!!! nastavak (31) a)

$$\left\{\frac{d}{dt}\left[(1-t^2)\frac{d}{dt}\right] - \left(\lambda + \frac{m^2}{1-t^2}\right)\right\}\Theta_1(t) = 0 \qquad (i)$$

$P_\ell^m(t)$

$$\Theta_1(t) = (1-t^2)^{\frac{|m|}{2}} S_*^{|m|}(t)$$

$$P_\ell^m(t) = (1-t^2)^{\frac{|m|}{2}} \left(\frac{d}{dt}\right)^{|m|} P_\ell(t)$$

$$S_*^{|m|}(t) = \left(\frac{d}{dt}\right)^{|m|} P_\ell(t)$$

motivacija:

1° $m \to -m$ ne povećava broj lin. nezav. rješenja, jer u jb.: je m pod kvadratom, već se rješenja za m i $-m$ lin. zavisna, tj. razlikuju se samo u nekom faktoru, recimo: $[1 + (m-|m|)C]$

2° asimptotsko ponašanje $\qquad t \in [-1,1]$

$\vartheta \to 0, \pi \Rightarrow t^2 \to 1 \Rightarrow 0 \le 1-t^2 \ll 1$

$$\Rightarrow \left\{\frac{d}{dt}\left[(1-t^2)\frac{d}{dt}\right] - \frac{m^2}{1-t^2}\right\}\Theta_1(t) = 0$$

$\Theta_1(t) \approx (1-t^2)^{\frac{|m|}{2}}$ aproximativno rješenje

$$\frac{d\Theta_1(t)}{dt} = -|m|t(1-t^2)^{\frac{|m|}{2}-1} \qquad -|m|t\left(\tfrac{|m|}{2}-1\right)(-2t)$$

$$\frac{d^2\Theta_1(t)}{dt^2} = -|m|(1-t^2)^{\frac{|m|}{2}-1} + |m|(|m|-2)t^2(1-t^2)^{\frac{|m|}{2}-2}$$

$$(1-t^2)\frac{d^2\Theta_1}{dt^2} - 2t\frac{d\Theta_1}{dt} - \frac{m^2}{(1-t^2)}\Theta_1 = -|m|(1-t^2)^{\frac{|m|}{2}} + |m|(|m|-2)t^2(1-t^2)^{\frac{|m|}{2}-1} + 2|m|t^2(1-t^2)^{\frac{|m|}{2}-1} - |m|^2(1-t^2)^{\frac{|m|}{2}-1} =$$

$$= -|m|(|m|+1)(1-t^2)^{\frac{|m|}{2}} \xrightarrow[|m|>0]{t^2\to 1} 0$$

$$(i) \to (1-t^2)\frac{d^2}{dt^2}S_*^{|m|}(t) - 2(|m|+1)t\frac{d}{dt}S_*^{|m|}(t) + \left[-\lambda - |m|(|m|+1)\right]S_*^{|m|}(t) = 0 \qquad (*)'$$

$$S_*^{|m|}(t) = \sum_{K=0}^{\infty} a_K t^K$$

$$\Rightarrow 2a_2 + \left[-\lambda - |m|(|m|+1)\right]a_0 = 0$$

$$6a_3 + \left[-\lambda - (|m|+1)(|m|+2)\right]a_1 = 0$$

$$(K+2)(K+1)a_{K+2} + \left[-\lambda - (|m|+K)(|m|+K+1)\right]a_K = 0$$

originalno!!!

$$S_*^{|m|}(t) = \sum_{K=0}^{\infty} a_K t^K$$

!!! ostavljeno

(14) a)

(**) $\Rightarrow$ $S_*^{|m|}(t)$ je red parnih ili neparnih potencija od t

$$S_*^{|m|}(\pm 1) = (a_0 + a_2 + a_4 + \dots + a_{2n} + \dots)$$

ili $= (\pm 1)(a_1 + a_3 + a_5 + \dots + a_{2n+1} + \dots)$

$$\frac{a_{K+2}}{a_K} = \frac{\lambda + (|m|+K)(|m|+K+1)}{(K+2)(K+1)} \xrightarrow{K \gg |m|} \frac{|m|+K}{(K+1)}$$

napomena: strože - bez nastojavanja

$$= \frac{\lambda}{(K+2)(K+1)} + \frac{(|m|+K)(|m|+K+1)}{(K+1)(K+2)}$$

$|x|<1$ $\quad (1-x)^{-|m|} = \sum_{K=0}^{\infty} \frac{|m|(|m|+1)\cdots(|m|+K-1)}{K!} x^K$ $\quad x=t^2$

: sjećanjem

$$(1-t^2)^{-|m|} = \sum_{K=0}^{\infty} \underbrace{\frac{|m|(|m|+1)\cdots(|m|+K-1)}{K!}}_{=C_{2K}} t^{2K} \qquad t=\pm 1 \;\Rightarrow\; = \sum_{K=0}^{\infty} C_{2K}$$

$$\frac{C_{2(K+1)}}{C_{2K}} = \frac{|m|+K}{K+1}$$

→ vidimo da za $t=\pm 1$ $S_*^{|m|}(t)$ prelazi u ∞ red samih koeficijenata koji je po omjeru susjednih koeficijenata sličan (u konverg. smislu) ∞ redu koeficijenata od $(1-t^2)^{-|m|}$

$\Rightarrow$ za $t = \pm 1$

$$\Theta_1(t) = (1-t^2)^{+\frac{|m|}{2}} \cdot S_*^{|m|}(t) \sim (1-t^2)^{\frac{|m|}{2}} \cdot (1-t^2)^{-|m|} = (1-t^2)^{-\frac{|m|}{2}} \to \infty$$

→ dakle samo regularno rješenje $\Theta_1(t)$ dolazi u obzir samo polinom za $S_*^{|m|}(t)$

- prekid ∞ reda $S_*^{|m|}(t)$ za: $a_K \neq 0 \quad a_{K+2} = 0 \quad \dots \quad a_{K+2s} = 0 \dots$

$$\lambda = -(|m|+K)(|m|+K+1) \qquad a_K \neq 0 \Rightarrow a_{K+2} = 0 \dots a_{K+2s} = 0 \dots$$

$$K^2 + (2|m|+1)K + (|m|^2 + |m| + \lambda) = 0$$

$$K_{1,2} = \frac{-(2|m|+1) \pm \sqrt{1-4\lambda}}{2}$$

$l \in \mathbb{Z}$

$m \in \mathbb{Z}$ & $K = 0,1,2,3,\dots \Rightarrow \sqrt{1-4\lambda} = 2l+1 \Rightarrow \lambda = -l(l+1) < 0$

$$\Rightarrow \quad K = \begin{cases} -|m|+l \\ -|m|-l-1 \end{cases} \quad \& \quad l = 0,1,2,3,\dots \quad \text{jer } \pm\sqrt{1-4\lambda} = \pm(2l+1)$$

ili $\quad K = -|m|+l \qquad l = 0, \pm 1, \pm 2, \pm 3, \dots$

tj. $\pm\sqrt{1-4\lambda} = \pm(2l+1)$ & $l = 0,1,2,\dots \Leftrightarrow +\sqrt{1-4\lambda} = (2l+1)$ & $l = 0, \pm 1, \pm 2, \dots$

$l = 0,1,2,\dots$ $\quad (2l+1) = 1,3,5,\dots$ $\quad -(2l+1) = -1,-3,-5,\dots$ (*)

$l = 0,1,2,\dots$ $\quad (2l+1) = 1,3,5,\dots$ $\quad l = -1,-2,-3,\dots$ $\quad (2l+1) = -1,-3,-5$ (*) $\quad l_1 = -l-1$

originalno!!!

→ $K \geq 0 \Rightarrow -|m|+l \geq 0 \Rightarrow \underline{|m| \leq l}$ (**)

$-|m|-l-1 \geq 0 \Rightarrow |m| \leq -l-1$ otpada za $l = 0,1,2,3,\dots$

$K \geq 0 \Rightarrow -|m|+l \geq 0$ & $l = 0, \pm 1, \pm 2, \pm 3, \dots \Rightarrow |m| \leq l$ ⇒ otpadaju vrijednosti $l = -1,-2,-3,\dots$

→ od dva linearno nezavisna rješenja za $S_*^{|m|}(t)$ (oo red parnih ili neparnih potencija) regularno je samo jedno i to ono koje se prekida

- to regularno rješenje je polinom $(l-|m|)$ stupnja parnih ili neparnih potencija ovisno o parnosti ili neparnosti razlike $(l-|m|)$

1° ako $(l-|m|)$ paran ⇒ oo red parnih potencija se prikida poslje $(l-|m|)$ člana dok oo red neparnih potencija se ne prekida

2° ako $(l-|m|)$ neparan ⇒ oo red neparnih potencija se prekida poslje $(l-|m|)$ člana dok red parnih potencija ostaje oo

→ za $\underline{\lambda = -l(l+1)}$ gdje $l = 0,1,2,\dots$ jbe. (*)' ⇔ (i) iz čega slijedi da je to regularno rješenje:

$$\underline{S_*^{|m|}(t) = \left(\frac{d}{dt}\right)^{|m|} P_l(t)}$$

$$\Rightarrow \underline{\Theta_1(t) = (1-t^2)^{\frac{|m|}{2}} S_*^{|m|}(t) = (1-t^2)^{\frac{|m|}{2}} \left(\frac{d}{dt}\right)^{|m|} P_l(t) = P_l^m(t)}$$

(**) ⇒ $m = -l, -l+1, \dots, -1, 0, 1, \dots l-1, l$

→ vidimo da u $\Theta_1(t)$ ne dolazi do izražaja da li je $m>0$ ili $m<0$ kao ni u dif. jbi. (i)

→ da li je $m>0$ ili $m<0$ dolazi do izražaja u faktoru

$$\underline{\phi(\varphi) = e^{im\varphi}}$$

zato i nismo pisali $\phi(\varphi) = e^{\pm im\varphi}$ kad i sam m je negativan

$t = \cos\vartheta$ $\quad Y(\vartheta,\varphi) = \Theta(\vartheta)\phi(\varphi)$ $\quad \Theta_1(\vartheta) = \Theta_1(t) = P_l^m(t) = P_l^m(\cos\vartheta)$

$$\Rightarrow \underline{Y_l^m(\vartheta,\varphi) = N_l^m P_l^m(\cos\vartheta) e^{im\varphi}} \qquad l = 0,1,2,\dots \quad m = 0, \pm 1, \dots \pm l$$

Sujeck II (605)

!!! ondamgre

$d\Omega = \sin\vartheta \, d\vartheta d\varphi$ — Kanjigram

$\vartheta = \pi \quad t = -1$

$\vartheta = 0 \quad t = 1$

$-dt \quad -\int_1^{-1} = \int_{-1}^{1}$

$$I^{mm'}_{ll'} = \int Y^m_l Y^{*m'}_{l'} d\Omega = \int_0^{2\pi}\int_0^{\pi} Y^m_l Y^{*m'}_{l'} d\varphi \sin\vartheta d\vartheta =$$

$$= N^m_l N^{*m'}_{l'} \underbrace{\int_0^{2\pi} e^{i(m-m')\varphi} d\varphi}_{2\pi\cdot\delta_{mm'}} \underbrace{\int_{-1}^{1} P^m_l(t) P^{m'}_{l'}(t) dt}_{\frac{2}{2l+1}\frac{(l+|m|)!}{(l-|m|)!}\delta_{ll'} \quad \text{za } m=m'} =$$

$$= N^m_l \cdot N^{*m'}_{l'} \frac{4\pi}{2l+1} \cdot \frac{(l+|m|)!}{(l-|m|)!} \delta_{mm'} \delta_{ll'}$$

zahtjev $I^{mm}_{ll} = 1 \Rightarrow |N^m_l|^2 = \frac{2l+1}{4\pi} \frac{(l-|m|)!}{(l+|m|)!}$

Def.1 $\Rightarrow$ $$Y^m_l(\vartheta,\varphi) = \sqrt{\frac{2l+1}{4\pi} \cdot \frac{(l-|m|)!}{(l+|m|)!}} P^m_l(\cos\vartheta) e^{im\varphi}$$

Def.2. $$P^m_l(t) = \frac{1}{2^l \cdot l!} (1-t^2)^{\frac{m}{2}} \left(\frac{d}{dt}\right)^{m+l} (t^2-1)^l \Rightarrow P^{-m}_l(t) = (-1)^m \frac{(l-m)!}{(l+m)!} P^m_l(t)$$

provjeri: $\Rightarrow |N^m_l|^2 = \frac{2l+1}{4\pi} \cdot \frac{(l-m)!}{(l+m)!}$ $\quad |N^{-m}_l|^2 = \frac{2l+1}{4\pi} \frac{(l+m)!}{(l-m)!}$

$$\Rightarrow Y^m_l(\vartheta,\varphi) = \eta^m_l \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} P^m_l(\cos\vartheta) e^{im\varphi}$$

$|\eta^m_l|^2 = 1$ — fazni faktor

$$\eta^m_l = 1, (-1)^m, (-1)^{l-m} \quad *)$$

$$Y^{-m}_l(\vartheta,\varphi) = \eta^{-m}_l \sqrt{\frac{2l+1}{4\pi}} \sqrt{\frac{(l+m)!}{(l-m)!}} P^{-m}_l(\cos\vartheta) e^{-im\varphi} = \eta^{-m}_l \sqrt{\frac{2l+1}{4\pi}} \sqrt{\frac{(l+m)!}{(l-m)!}} \cdot (-1)^m \frac{(l-m)!}{(l+m)!} P^m_l(\cos\vartheta) e^{-im\varphi}$$

$$= \frac{\eta^{-m}_l}{\eta^{*m}_l} (-1)^m \eta^{*m}_l \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} P^m_l(\cos\vartheta) e^{-im\varphi}$$

$$Y^{-m}_l(\vartheta,\varphi) = \frac{\eta^{-m}_l}{\eta^{*m}_l} (-1)^m Y^{*m}_l(\vartheta,\varphi) \overset{*)}{=} (-1)^m Y^{*m}_l(\vartheta,\varphi)$$

Сферна ј-ба. стр 31

$$\frac{d^2R}{ds^2} + \frac{2}{s}\frac{dR}{ds} + \left(1 + \frac{\lambda}{s^2}\right)R(s) = 0 \quad (*)$$

за $R(s) = \frac{z_p(s)}{\sqrt{s}}$ и Бесселова диф. ј-ба

$$z_p''(s) + \frac{1}{s}z_p' + \left(1 - \frac{p^2}{s^2}\right)z_p(s) = 0$$

$$\rightarrow R'' + \frac{2}{s}R' + \left(1 + \frac{\frac{1}{4} - p^2}{s^2}\right)R = 0$$

$$\Rightarrow \lambda = \frac{1}{4} - p^2 \qquad R(s) = \frac{J_p(s)}{\sqrt{s}}$$

за $s \ll 1 \Rightarrow 1 + \frac{\lambda}{s^2} \approx \frac{\lambda}{s^2}$

$$(*) \rightarrow \frac{d^2R}{ds^2} + \frac{2}{s}\frac{dR}{ds} + \frac{\lambda}{s^2}R = 0 \Rightarrow R(s) = As^{l_1} + Bs^{l_2}$$

$$l(l-1) + 2l = \lambda \Rightarrow \boxed{-\lambda = l(l+1)}$$

$$p = \sqrt{\frac{1}{4} - \lambda} = \pm\left(l + \frac{1}{2}\right)$$

$$\Rightarrow R(s) = \frac{J_{(l+\frac{1}{2})}(s)}{\sqrt{s}} \qquad \text{за } s \ll 1 \qquad R(s) = \sqrt{\frac{\pi}{2}} \cdot j_l(s)$$

$$j_l(s) = \sqrt{\frac{\pi}{2s}} \cdot J_{(l+\frac{1}{2})}(s) \xrightarrow{s \ll 1} \frac{s^l}{(2l+1)!!}$$

$$\xrightarrow{s \gg 1} \frac{\sin\left(s - l\frac{\pi}{2}\right)}{s}$$

*) uz (3) a) $t \in [-1, 1]$

asimptotsko ponašanje: $\vartheta \to 0, \pi$ $t^2 \to 1$

$$\left\{ \frac{d}{dt}\left[(1-t^2)\frac{d}{dt} \right] - \frac{m^2}{1-t^2} \right\} \Theta_1^{(m)}(t) = 0 \qquad \underline{0 \leq 1-t^2 \ll 1}$$

aprox. rješ. $\Theta_1^{(m)}(t) \sim (1-t^2)^{-\frac{m}{2}}$

$$\frac{d\Theta_1^{(m)}}{dt} = m t (1-t^2)^{-\frac{m}{2}-1}$$

$$\frac{d^2\Theta_1^{(m)}}{dt^2} = m(1-t^2)^{-\frac{m}{2}-1} + m(m+2)t^2(1-t^2)^{-\frac{m}{2}-2}$$

$$\Rightarrow \frac{d}{dt}\left[(1-t^2)\frac{d\Theta_1^{(m)}}{dt} \right] - \frac{m^2}{1-t^2}\Theta_1^{(m)}(t) =$$

$$= m(1-t^2)^{-\frac{m}{2}} - m^2(1-t^2)(1-t^2)^{-\frac{m}{2}-1}$$

$$= m(1-t^2)^{-\frac{m}{2}} - m^2(1-t^2)^{-\frac{m}{2}}$$

$$= \underline{m(1-m)(1-t^2)^{-\frac{m}{2}}}$$

$t^2 \to 1 \longrightarrow 0$ za $\underline{m < 0}$ $m = -1, -2, -3, \ldots$

asimptotsko rješenje

$\oint\oint\oint_H = s\,pas$

$\Theta(\vartheta) = \sin^{-m}\vartheta \; S_\ell^{(m)}(\cos\vartheta)$

$\Theta_1(t) = \left(\sqrt{1-t^2}\right)^{-m} \cdot S_\ell^{(m)}(t)$

$\vartheta = 0, \pi \Rightarrow t^2 \to 1$

$\left(\lambda + \frac{m^2}{1-t^2}\right)$

as. impd. pentru $\vartheta \to 0, \pi \Rightarrow t^2 \to 1$

$\frac{m^2}{1-t^2}\,\Theta_1(t) = 0 \Rightarrow$

$$(1-t^2)\frac{d^2\Theta}{dt^2} - 2t\frac{d\Theta}{dt} - \left(\lambda + \frac{m^2}{1-t^2}\right)\Theta = 0$$

$t^2 \to 1$

$$-2t\frac{d\Theta}{dt} - \left(\lambda + \frac{m^2}{1-t^2}\right)\Theta = 0$$

$$-2t\frac{d\Theta}{dt} - \frac{m^2}{1-t^2}\Theta = 0$$

**) na (31a)

za $m>0$ $|x|<1$

$$(1-x)^{-m} = \sum_{k=0}^{\infty} \frac{m(m+1)\cdots(m+k-1)}{k!} x^k = 1 + mx + \frac{m(m-1)}{2!}x^2 + \dots$$

$$(1-t^2)^{-\frac{m}{2}} = \sum_{k=0}^{\infty} \underbrace{\frac{m(m+2)\cdots(m+2(k-1))}{2^k \cdot k!}}_{\| C_{2k}} t^{2k}$$

$$\frac{C_{2(k+1)}}{C_{2k}} = \frac{m+2k}{2(k+1)} \xrightarrow[k \gg |m|]{k \gg m > 0} 1$$

za $m<0$ $|x|\leq 1$

$$\frac{1}{2^k}(-1)^k \, m(m+2)\cdots[m+2(k-1)]$$
$$\left(-\tfrac{m}{2}\right)\left[-\tfrac{m}{2}-1\right]\cdots\left[-\tfrac{m}{2}-(k-1)\right]$$

$$(1-x)^{m'} = \sum_{k=0}^{m'\geq 0} (-1)^k \frac{m'(m'-1)\cdots(m'-k+1)}{k!} x^k \qquad m' = -\frac{m}{2} > 0 \text{ za } m<0$$

$$(1-t^2)^{-\frac{m}{2}} = \sum_{k=0}^{\infty} \underbrace{\frac{m(m+2)\cdots(m+2(k-1))}{2^k \cdot k!}}_{\| C_{2k}} t^{2k}$$

$$\frac{C_{2(k+1)}}{C_{2k}} = \frac{m+2k}{2(k+1)} \xrightarrow[m<0]{k \gg |m|} 1$$

Prekid reda $S_l^{(m)}(t)$ ako za neki K

$$\lambda = -(m-K)(m-K-1) \qquad a_K \neq 0 \quad \cdots \quad a_{K+2} = 0$$

$K = 2s$ ili $K = 2s_1 + 1$

$$K^2 + (-2m+1)K + (m^2 - m + \lambda) = 0$$

$$K_{1,2} = \frac{(2m-1) \pm \sqrt{1-4\lambda}}{2}$$

$m \in Z \qquad K = \underline{0}, 1, \underline{2}, 3, \underline{4}, \ldots$ $\qquad 2s = 0, 2, 4, \ldots$ $\qquad 2s_1+1 = 1, 3, 5, \ldots$

$\Rightarrow \sqrt{1-4\lambda} = 2l+1 \quad = 1, 3, 5, 7, \ldots$

$l = 0, 1, 2, 3, \ldots$ jer $\pm\sqrt{1-4\lambda}$

$\lambda = -l_1(l_1+1) = -l(l+1)$

$K = m+l = m-l_1-1$

$$\lambda = -l(l+1) \qquad \underline{l = 0, 1, 2, 3, \ldots}$$

nepotrebno $l_1 = -1, -2, -3, \ldots$ jer s korespodencija $l_1 = -l-1$

$$\Rightarrow K = \begin{cases} + \{ m+l \} \geq 0 \Rightarrow m \geq -l \\ - \{ m-l-1 \} \geq 0 \Rightarrow m \overset{\text{ili}}{\geq} l+1 \end{cases}$$

$(m+l)-(2l+1)$

dvojesenja u odnosu na redove parnih i neparnih potencija

$(m+l) \geq 0$

$m \geq -l$ $\quad m+l = 2s$ red parnih potencija se prekida

$m+l = 2s_1+1$ red neparnih potencija se prekida

$(m+l) \geq 2l+1$

$m \geq l+1$ $\quad -(l-1)$

$m+l = 2s$ red neparnih potencija se prekida

$m+l = 2s_1+1$ red parnih potencija se prekida

pridruž. Legendr. polinom $S_*^{(m)} = \left(\frac{d}{dt}\right)^m S_\ell^{(0)}(t)$

$t = \cos\vartheta$

$$P_\ell^m(t) = \left(\sqrt{1-t^2}\right)^m S_*^{(m)} = (1-t^2)^{\frac{m}{2}} \frac{d^m}{dt^m} S_\ell^{(0)}(t) = (1-t^2)^{\frac{|m|}{2}} \left(\frac{d}{dt}\right)^{|m|} P_\ell(t)$$

Rodrigez-formula

$$P_\ell(t) = S_\ell^{(0)}(t) = \frac{(-1)^\ell}{\ell!\, 2^\ell} \frac{d^\ell}{dt^\ell}(1-t^2)^\ell = \frac{1}{2^\ell \cdot \ell!}\left(\frac{d}{dt}\right)^\ell (t^2-1)^\ell$$

običan Legendr. polinom ℓ-tog stupnja

da valna fja. ne iščezava $\left(\frac{d}{dt}\right)^{|m|}(a_\ell t^\ell + \dots)$

$\Rightarrow |m| \le \ell$ (*) (pogledaj (**) (31) g)

iz $e^{im(\varphi+2\pi)} = e^{im\varphi} \Rightarrow e^{im2\pi} = 1 \Rightarrow m = \underbrace{0, \pm 1, \pm 2, \dots \pm \ell}_{2\ell+1}$

(*)

ročsmo ih sreli

Vidjet ćemo $M^2 = \hbar^2 \ell(\ell+1)$

$M_z = \hbar m$

Paritet

- promatramo ponašanje fje. $F(x,y,z)$

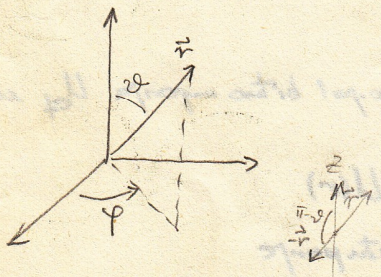
za $\vec{r} \to -\vec{r}$ $(x \to -x)$

- na primjeru rješ. Schrödingera za sfernosim. potencijal

$$u(r,\vartheta,\varphi) = R(r)\, Y(\vartheta,\varphi)$$

umjesto $\vec{r} \to -\vec{r}$ tj. $x \to -x$ $y \to -y$ $z \to -z$

lijevi sustav $\to$ desni



$r \to r$

$\varphi \to \varphi + \pi$

$\vartheta \to \pi - \vartheta$

relevantna samo promjena Kugline fje. $Y(\vartheta,\varphi)$

$\cos\vartheta \to \cos(\pi-\vartheta) = -\cos\vartheta \Rightarrow t \to -t$

$$\Rightarrow P_\ell^m \to (-1)^{\ell+m} P_\ell^m$$

$$e^{im\varphi} \to e^{im(\varphi+\pi)} = e^{im\varphi} \cdot (-1)^m$$

$$P_\ell^m(t) = \frac{1}{2^\ell \ell!}(1-t^2)^{\frac{|m|}{2}} \cdot \left(\frac{d}{dt}\right)^{|m|+\ell} (t^2-1)^\ell$$

$$P_\ell^m(-t) = (-1)^{|m|+\ell} P_\ell^m(t)$$

$$\text{jer } \left(\frac{d}{dt}\right)^{|m|+\ell} = (-1)^{|m|+\ell}\left(\frac{d}{d(-t)}\right)^{|m|+\ell}$$

$Y_l^m = c_{lm} P_l^m e^{im\varphi}$ $\quad P_l^m \to (-1)^{l+m} P_l^m$ $\quad e^{im\varphi} \to (-1)^m e^{im\varphi}$

$\Rightarrow$ $\boxed{Y_l^m(\vartheta,\varphi) \xrightarrow{\vec{r}\to-\vec{r}} (-1)^l Y_l^m(\vartheta,\varphi)}$

stanja s $\begin{cases} \text{pozit. paritetom} & \text{za } l\text{-paran} \\ \text{negat. paritetom} & \text{za } l\text{-neparan} \end{cases}$

$U = U(r) \qquad u = R(r)\,Y(\vartheta,\varphi) \Rightarrow \frac{1}{r}\frac{d^2}{dr^2}(rR) + \left[\frac{2m}{\hbar^2}(E-U(r)) + \frac{\lambda}{r^2}\right] R(r) = 0$

$\Lambda Y = \lambda \cdot Y \qquad \lambda = -l(l+1) \qquad l = 0,1,2,\ldots$

$$\boxed{\left[\frac{d^2}{dr^2} + \frac{2m}{\hbar^2}(E - U_{ef}(r))\right](rR(r)) = 0} \qquad (*)$$

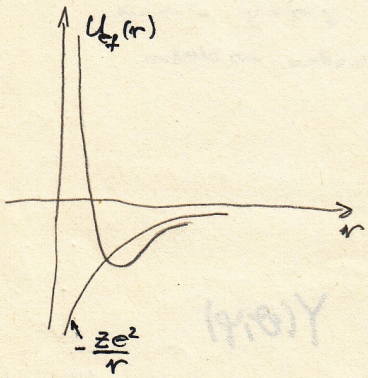
$$\boxed{U_{ef}(r) = U(r) + \underbrace{\frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}}_{\text{centrifugalni potencial} \;=0 \text{ za } l=0} \qquad l = 0,1,2,3,\ldots}$$

$(*)$ liči Schröd. jb. ugodnodim. problema $\frac{d^2u}{dx^2} + \frac{2m}{\hbar^2}(E-U(x))u = 0$

za $l=0$ nema razlike $U_{ef}(r) = U(r)$

→ Ilustracija: - promjena potenc. kod gib. čestice u Coulomb. polju

$$\underline{U(r) = -\frac{ze^2}{r}} \Rightarrow \underline{U_{ef}(r)} = -\frac{ze^2}{r} + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}$$



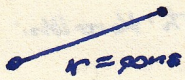
za $l \neq 0$ centrif. potencijal bitno mijenja U_{ef} u ishodištu

r - velik $\quad U_{ef}(r) \to U(r)$

r - malo $\quad$ velike odstupanje

Rotator

- čestica u stalnoj udalj. giba se oko centra koji je privlači:



$\Rightarrow \quad u(r,\vartheta,\varphi) = \underbrace{U(r)}_{\text{const.}} \cdot Y_l^m(\vartheta,\varphi) \Rightarrow$

$\frac{d^2}{dr^2}(rR(r)) = 0$

$\Rightarrow E - U_{ef}(r) = 0$

$u(\vartheta,\varphi) = \text{const.}\ Y_l^m(\vartheta,\varphi)$ - kuglina fja.

$(*) \Rightarrow E = U(r) + \underbrace{\frac{\hbar^2}{2m}\cdot\frac{l(l+1)}{r^2}}_{E_{rot}}$

$U(r)=0 \Rightarrow E = E_{rot}$

$\Rightarrow M^2 = \hbar^2 l(l+1)$

Kompariramo s klas. izrazom $E_{rot} = \frac{M^2}{2J}$ & $J = mr^2$

$E_{rot} = \frac{mv^2}{2} = \frac{m^2 r^2 v^2}{2m\cdot mr^2} = \frac{(mrv)^2}{2J}$

dokazano za slučaj rotatora

Vodikov atom

- rješavali smo u okviru Bohr-ove teorije, ali neprovilan pristup (staza)

  historijski: istovremeno Pauli na osnovu Heisenb. teorije & Schröd. kada objavljuje valnu teoriju (siječanj 1926)

$U(r) = -\frac{Ze^2}{r} \qquad H = \frac{p^2}{2m} - \frac{Ze^2}{r}$

→ približno: $E_0 \simeq \frac{(\Delta p)^2}{2m} - \frac{Ze^2}{\Delta r}$ $\quad p_r = m\dot{r}$

zbog $\Delta p_r \cdot \Delta r \simeq \hbar$

$E_0 \simeq \frac{\hbar^2}{2m(\Delta r)^2} - \frac{Ze^2}{\Delta r}$

Kolika je neizvjesnost Δr koja će nas dovesti na stanje min. energije

$\frac{dE_0}{d(\Delta r)} = -\frac{\hbar^2}{m(\Delta r)^3} + \frac{Ze^2}{(\Delta r)^2} = 0 \Rightarrow \Delta r = \frac{\hbar^2}{mZe^2}$ - promjena po realnoj veličini

$E_0 \simeq \frac{\hbar^2 \cdot m^2 Z^2 e^4}{2m\,\hbar^4} - \frac{Ze^2 \cdot m Ze^2}{\hbar^2} = -\frac{mZ^2e^4}{2\hbar^2}$ - real. veličine

→ u Bohr-ovoj (neprovilan pristup - staza) teoriji dobivamo dobar rezultat za energ. (eksp. potvrda - ali ne za el. i magn. polje → cijepanje linija)

$E_n = -\frac{mZ^2e^4}{2\hbar^2 n^2}$

1° Problem 2 tijela → (rješiti) Schröd. jbu. uz relativnu (masa μ) koordinatu $r = |\vec{r}_2 - \vec{r}_1|$ (elektron)
i za koord. težišta (masa M) (Klas. fizika)

$$\frac{1}{\mu} = \frac{1}{m} + \frac{1}{M}$$

u slučaju ako želimo biti korektni: ali za elektron pišemo m za μ

pretpostavimo da smo riješili taj dio problema

2° Kepler-ov problem – Kakva je E elektr. koji se giba oko jezgre (*)
(Klas. fizika)

$E < 0$ elipsa ⇔ (odgovara) vezano stanje u Kvantnoj fizici (bit će kvantizirano)

$E = 0$ parabola
$E > 0$ hiperbola } čestica samoprobiva kraj jezgre

Schröd. jba:

$$\left[\frac{d^2}{dr^2} - \frac{2m}{\hbar^2}|E| + \frac{2m}{\hbar^2}\frac{Ze^2}{r} - \frac{l(l+1)}{r^2}\right] \underbrace{rR(r)}_{U_1(r)} = 0 \quad i) \Big/ \cdot \frac{\hbar^2}{2m|E|} \cdot \frac{1}{4}$$

$$\frac{d\phi}{dr} = \frac{d\phi}{d\rho}\frac{d\rho}{dr} = \frac{d\phi}{d\rho}\cdot\frac{2}{\hbar}\sqrt{2m|E|}$$

$$\frac{d^2\phi}{dr^2} = \frac{2}{\hbar}\sqrt{2m|E|}\,\frac{d^2\phi}{d\rho^2}\cdot\frac{d\rho}{dr} = \frac{d^2\phi}{d\rho^2}\cdot\frac{4}{\hbar^2}(2m|E|)$$

→ varijable bez dimenzija:

$$\frac{1}{\hbar} = \frac{\hbar k}{\hbar} = \frac{2\pi}{\lambda}$$

$$\rho = r\cdot\frac{2}{\hbar}\sqrt{2m|E|}$$

& Bohr-ov oblik $|E| = \dfrac{mZ^2e^4}{2\hbar^2 n^2}$, gdje tek račun treba dati da je n cjelobrojan – glavni kvantni broj

$$\rho = r\,\frac{2}{\hbar^2}\frac{mZe^2}{n} = \frac{2rZ}{n}\cdot\frac{me^2}{\hbar^2}$$

Bohr. teorija: $r_n = \dfrac{\hbar^2 n^2}{mZe^2} \Rightarrow r_1 = \dfrac{\hbar^2}{Zme^2}$

$$\Rightarrow \rho = \frac{2rZ}{n r_0} \left(= \frac{2Z}{nr_0}\cdot r\right) \qquad r_0 = \frac{\hbar^2}{me^2}$$

$$\frac{Ze^2}{4|E|}\cdot\frac{2}{\hbar}\sqrt{2m|E|}\,\frac{1}{\rho} = \frac{1}{\rho}\cdot\frac{Ze^2\sqrt{m}}{\hbar\sqrt{|E|}2} = n$$

$$-\frac{l(l+1)}{\left(r\cdot\frac{2}{\hbar}\sqrt{2m|E|}\right)^2}$$

$$U_1(r) = rR(r) = \frac{nr_0}{2Z}\cdot\rho\cdot R\left(\frac{nr_0}{2Z}\cdot\rho\right) = U(\rho)$$

$$\Rightarrow \left[\frac{d^2}{d\rho^2} - \frac{1}{4} + \frac{n}{\rho} - \frac{l(l+1)}{\rho^2}\right] U(\rho) = 0 \quad ii)$$

zapravo: $R(r) = C_1\,\dfrac{U(\rho)}{r}$

treba riješiti → asimptotsko ponašanje za $\rho \gg$ & $\rho \ll$

1) $\rho \to \infty$

$$v'' - \frac{1}{4} v = 0 \quad \Rightarrow \quad v(\rho) = \begin{cases} e^{-\frac{\rho}{2}} \\ e^{\frac{\rho}{2}} \end{cases}$$

ne zadovolji uvjet regularnosti (konačnost) za $\rho \to \infty$

$$v = C e^{-\frac{\rho}{2}}$$

2) $\rho \to 0$ prevladava centrif. potencijal

$$v_{(\rho)}'' - \frac{l(l+1)}{\rho^2} v_{(\rho)} = 0$$

$v(\rho) = \rho^n \Rightarrow n(n-1) = l(l+1)$

$n = l+1$

$n = -l$

$$\Rightarrow v(\rho) = \begin{cases} \rho^{l+1} \\ \rho^{-l} \end{cases}$$

odgovara za $l = 0, 1, 2, \ldots$

neodgovara za $l = 1, 2, 3, \ldots$ za $l = 0$ odgovara

$r \to 0 \Rightarrow \rho \to 0 \quad \rho = e^{+t} \quad v(\rho) = v_1(t)$

$\frac{d}{d\rho} = \frac{d}{dt}\frac{1}{\rho} \qquad \frac{d^2}{d\rho^2} = \frac{d}{d\rho}\left(\frac{1}{\rho}\frac{d}{dt}\right) = -\frac{1}{\rho^2}\frac{d}{dt} + \frac{1}{\rho^2}\frac{d^2}{dt^2}$

$\Rightarrow -\frac{1}{\rho^2}\dot{v}_1 + \frac{1}{\rho^2}\ddot{v}_1 - \frac{l(l+1)}{\rho^2} v = 0$

$\ddot{v}_1 - \dot{v}_1 - l(l+1) v = 0$

$\lambda^2 + 4l + 1$

$v_0 = e^{rt} \qquad r_{1/2} = \frac{1 \pm \sqrt{1 + 4l(l+1)}}{2}$

$v_1(t) = A e^{(l+1)t} + B e^{-lt} \qquad \frac{1 \pm (2l+1)}{2}$

$v(\rho) = A \rho^{l+1} + B \rho^{-l}$

→ rješ. radijalne Schröd. jbe.

$$v(\rho) = e^{-\frac{\rho}{2}} \cdot \rho^{l+1} L(\rho)$$

← Laguerre-ovi pridruženi polinomi - pridruženi pridruž. fja

Supek II 580.

nove indeks n, l

bitno!!!

ne smije promijeniti asimptotsko ponašanje za $\rho \to 0$ & $\rho \to \infty$

$$v'(\rho) = -\frac{1}{2} e^{-\frac{\rho}{2}} \cdot \rho^{l+1} L(\rho) + (l+1) e^{-\frac{\rho}{2}} \cdot \rho^{l} L(\rho) + e^{-\frac{\rho}{2}} \cdot \rho^{l+1} L'(\rho)$$

$$v''(\rho) = L(\rho)\left[\frac{1}{4} e^{-\frac{\rho}{2}} \rho^{l+1} - \frac{1}{2}(l+1) e^{-\frac{\rho}{2}} \rho^{l} - \frac{1}{2}(l+1) e^{-\frac{\rho}{2}} \rho^{l} + (l+1) l\, e^{-\frac{\rho}{2}} \rho^{l-1}\right]$$

$$+ L'(\rho)\left[-\frac{1}{2} e^{-\frac{\rho}{2}} \rho^{l+1} + (l+1) e^{-\frac{\rho}{2}} \rho^{l} + \frac{1}{2} e^{-\frac{\rho}{2}} \rho^{l+1} + (l+1) e^{-\frac{\rho}{2}} \rho^{l}\right] + e^{-\frac{\rho}{2}} \cdot \rho^{l+1} \cdot L''(\rho)$$

$$= L(\rho)\left[\frac{1}{4} e^{-\frac{\rho}{2}} \rho^{l+1} - (l+1) e^{-\frac{\rho}{2}} \rho^{l} + (l+1) l\, e^{-\frac{\rho}{2}} \rho^{l-1}\right]$$

$$+ L'(\rho)\left[-e^{-\frac{\rho}{2}} \rho^{l+1} + 2(l+1) e^{-\frac{\rho}{2}} \rho^{l}\right] + e^{-\frac{\rho}{2}} \rho^{l+1} L''(\rho)$$

$$v''(\rho) + \left[-\frac{1}{4} e^{-\frac{\rho}{2}} \rho^{l+1} + n\, e^{-\frac{\rho}{2}} \rho^{l} - l(l+1) e^{-\frac{\rho}{2}} \rho^{l-1}\right] L(\rho) = 0 \qquad / \cdot \frac{e^{\frac{\rho}{2}}}{\rho^l}$$

$$\Rightarrow \rho \cdot L''(\rho) + L'(\rho)\left[2(l+1) - \rho\right] + L(\rho)\left[n - l - 1\right] = 0$$

$$\boxed{\rho L''(\rho) + \left[2(l+1) - \rho\right] L'(\rho) + (n - l - 1) L(\rho) = 0}$$

pretp: $L(s) = \sum_{k=0}^{n_r} a_k s^k$ $\quad L' = \sum_{k=1}^{n_r} k a_k s^{k-1}$ $\quad L'' = \sum_{k=2}^{n_r} k(k-1) a_k s^{k-2}$

$$\sum_{k=2}^{n_r} k(k-1) a_k s^{k-1} + \sum_{k=1}^{n_r} 2(l+1) k a_k s^{k-1} + \sum_{k=1}^{n_r} -k a_k s^k + \sum_{k=0}^{n_r} (n-l-1) a_k s^k = 0$$

$k \leftarrow k+1$

$$\sum_{k=1}^{n_r-1} k(k+1) a_{k+1} s^k + \sum_{k=0}^{n_r-1} 2(l+1)(k+1) a_{k+1} s^k + \sum_{k=1}^{n_r} -k a_k s^k + \sum_{k=0}^{n_r} (n-l-1) a_k s^k = 0$$

$$\sum_{k=1}^{n_r-1} s^k \left\{ a_{k+1}\left[k(k+1) + 2(l+1)(k+1)\right] - a_k\left[k - n + (l+1)\right] \right\} +$$

$$+ 2(l+1) a_1 - n_r a_{n_r} s^{n_r} + (n-l-1) a_{n_r} s^{n_r} + (n-l-1) a_0 = 0$$

za $\forall s \Rightarrow$

$$a_{k+1} = \frac{k+l+1-n}{(k+1)\left[k+2(l+1)\right]} a_k \quad (i)$$

$k = 1, \dots (n_r - 1)$ $\quad$ $n_r \in N \cup \{0\}$

$k = 0, 1, 2, \dots (n_r - 1)$ $\quad$ $l = 0, 1, 2, \dots$

n - nezna mo još

$$2(l+1) a_1 + (n-l-1) a_0 = 0$$

$$(n-l-1-n_r) a_{n_r} = 0 \quad (i)'$$

→ za $k = n_r$ polinom se mora prekinuti, tj. n_r mora biti konačan

dokaz:

$$\frac{a_{k+1}}{a_k} \xrightarrow[k\to\infty]{} \frac{1}{k} \quad \text{jer} \quad e^s = \sum_{k=0}^{\infty} \frac{1}{k!} s^k \quad \text{i} \quad \frac{\frac{1}{(k+1)!}}{\frac{1}{(k)!}} = \frac{1}{k+1} \overset{k\to\infty}{\approx} \frac{1}{k}$$

dakle, ako bi dopustili da $n_r \to \infty$ tada bi se $L(s)$ u smislu konvergencije ponašao kao e^s, pa bi bilo

$$V(s) = s^{l+1} \cdot e^{-\frac{s}{2}} \cdot L(s) \xrightarrow[s\gg]{} s^{l+1} e^{-\frac{s}{2}} \cdot e^s = e^{\frac{s}{2}} \cdot s^{l+1} \xrightarrow[s\to\infty]{} \infty$$

za $l = 0, 1, 2, \dots$ čak nezavisno od n

uvjet regularnosti ⇒ n_r konačan

$$u_{nlm}(r,\vartheta,\varphi) = R_{nl}(r)\, Y_l^m(\vartheta,\varphi)$$

$\frac{1}{\rho} = \frac{r_0 n}{2Z}\frac{1}{r}$

$$R_{nl}(r) = C_1 \frac{e^{-\frac{\rho}{2}} \cdot \rho^{l+1} L(\rho)}{r} \qquad \rho = \frac{2Z}{r_0 n}\cdot r \qquad r_0 = \frac{\hbar^2}{me^2}$$

$$R_{nl}(r) = \frac{e^{-\frac{Z}{r_0 n}\cdot r}\cdot\left(\frac{2Z}{r_0 n}\right)^{l+1}\cdot r^{l+1} L\left(\frac{2Z}{r_0 n}\cdot r\right)}{r}$$

$$R_{nl}(r) = C_1\left(\frac{2Z}{r_0 n}\right)^{l+1}\cdot e^{-\frac{Z}{r_0 n}\cdot r}\cdot r^{l+1}\cdot L\left(\frac{2Z}{r_0 n}\cdot r\right)$$

$$\int \psi^* \cdot \psi \, d\tau = 1 \Rightarrow \int u_{nlm}^2(r,\vartheta,\varphi)\, d\tau = 1$$

$d\tau = dx\,dy\,dz$

$dx\,dy\,dz = \left|\frac{\partial(x,y,z)}{\partial(r,\vartheta,\varphi)}\right| dr\,d\vartheta\,d\varphi$, $r^2\sin\vartheta$

$$\int_0^\infty R_{nl}^2(r) r^2 dr \int_0^{2\pi}\int_0^{\pi} Y_l^{m\,2}(\vartheta,\varphi)\, d\varphi \sin\vartheta\, d\vartheta = 1$$

$d\varphi\sin\vartheta\,d\vartheta = d\Omega$

$= 1$ iii) za (31)

$$\Rightarrow \int_0^\infty R_{nl}^2(r) r^2 dr = 1$$

Hao i Supek II 90.

ili $R_{nl}(r) = R_{nl}\left(\frac{r_0 n}{2Z}\cdot\rho\right) = R_{nl_1}(\rho) = \frac{2Z}{r_0 n} C_1 \frac{e^{-\frac{\rho}{2}}\cdot\rho^{l+1} L_{n+l}^{2l+1}(\rho)}{\rho} =$

Hao i Supek I str. 90. $\longrightarrow$ $= \underbrace{\frac{2Z}{r_0 n}\cdot C_1}_{=C} e^{-\frac{\rho}{2}}\cdot\rho^l L_{n+l}^{2l+1}(\rho) = \frac{2Z}{r_0 n} C_1 e^{-\frac{\rho}{2}}\cdot\rho^{\frac{p-1}{2}} L_{n+p}^{p}(\rho)$

$m+p$

$$R_{nl}(r) = \underbrace{\frac{2Z}{r_0 n}\cdot C_1}_{C} R_{n+p}^{p}(\rho)$$

$p = 2l+1$, $n+p = n+l$ i $\rho = \frac{2Z}{r_0 n} r$

$$\int_0^\infty R_{nl}^2(r)\, r^2 dr = 1 \qquad R_{nl}(r) = C R_{n+l}^{2l+1}(\rho) \qquad \rho = \frac{2Z}{nr_0}\cdot r$$

$$\Rightarrow \quad 1 = |C|^2 \left(\frac{nr_0}{2Z}\right)^3 \int_0^\infty \left(R_{n+l}^{2l+1}(\rho)\right)^2 \rho^2 d\rho$$

$$|C|^2 = \left(\frac{2Z}{nr_0}\right)^3 \cdot \frac{n_r!}{2n\,[(n+l)!]^3}$$

uzmimo C realnu negativnu veličinu

$$C = -\sqrt{\left(\frac{2Z}{nr_0}\right)^3 \frac{n_r!}{[(n+l)!]^3 2n}} \qquad n = n_r + l + 1$$

uz (35) a)

$$L(\varrho) = \sum_{k=0}^{n_r} a_k \varrho^k$$

$$a_{k+1} = \frac{k+l+1-n}{(k+1)(k+2(l+1))} a_k \qquad k = 0, 1, 2, \ldots (n_r - 1)$$

$n = n_r + l + 1$ $\qquad$ a_0 - odredit iz normiranja

$$a_{k+1} = \frac{k - n_r}{(k+1)[k+2(l+1)]} a_k \qquad k = 0, 1, 2, \ldots (n_r - 1)$$

$$\Rightarrow L_{n_r\, l}(\varrho) = \sum_{\substack{k=0 \\ (n+l)-(2l+1) \\ n-(l+1) \geq 0}}^{n_r \geq 0} a_k \varrho^k$$

$k = 0, 1, 2, \ldots [(n+l)-(2l+1)]$

$$a_{k+1} = \frac{k + (2l+1) - (n+l)}{(k+1)[(k+1)+(2l+1)]} a_k$$

ili: $$L^{2l+1}_{n+l}(\varrho) = \sum_{k=0} a_k \varrho^k$$

$$a_{k+1} = \frac{k+l+1-n}{(l+1)[k+2(l+1)]} a_k$$

$k = 0, 1, \ldots [n-(l+1)]$

Supek 581:

obični Laguerre-polinomi:

$$L_n(\varrho) = \sum_{k=0}^{n} \frac{(-1)^k n!}{k!} \binom{n}{k} \varrho^k = e^{\varrho} \left(\frac{d}{d\varrho}\right)^n \varrho^n e^{-\varrho}$$

pridruženi Laguerre polinomi:

$$L^p_{m+p}(\varrho) \overset{\text{def.}}{=} \left(\frac{d}{d\varrho}\right)^p L_{m+p}(\varrho)$$

$$L^0_m(\varrho) = L_m(\varrho) \qquad p = 0, 1, 2, \ldots \quad m = 0, 1, 2, \ldots$$

$\Rightarrow$ jba. $[\varrho(\frac{d}{d\varrho})^2 + (p+1-\varrho)\frac{d}{d\varrho} + m] L^p_{m+p}(\varrho) = 0$

$\Rightarrow$ $p = 2l+1$, $m+p = n+l$ $\Rightarrow$ $m = n-l-1$

$\Rightarrow$ jba. sa (34) $[\varrho(\frac{d}{d\varrho})^2 + \underbrace{[2(l+1)-\varrho]}_{(2l+1)+1-\varrho}\frac{d}{d\varrho} + \underbrace{(n-l-1)}_{k}] L^{2l+1}_{n+l}(\varrho) = 0$

$k = (n+l)-(2l+1)$

L^p_{m+p}

$L^0_0 = 1$ $\quad L^1_1 = -1$

$L^0_1 = -r+1$ $\quad L^1_2 = 2r-4$ $\quad L^2_2 = 2$

$L^0_2 = r^2 - 4r + 2$ $\quad L^1_3 = -3r^2+18r-18$ $\quad L^2_3 = -6r+18$ $\quad L^3_3 = -6$

$L^0_3(r) = -r^3+9r^2-18r+6$

Laguerre-ove pridružene fje:

$$R^p_{m+p}(\rho) = e^{-\frac{\rho}{2}} \cdot \rho^{\frac{p-1}{2}} L^p_{m+p}(\rho)$$

Schiff II 58.

$m = n+l-2l-1 = n-l-1$

$p = 2l+1$

$$\int_0^\infty \left(R^p_{m+p}(\rho)\right)^2 \rho^2 d\rho = \frac{2m+p+1}{m!} \underbrace{[(m+p)!]^3}_{(n+l)!}$$

$$\int_0^\infty \left(R^{2l+1}_{n+l}(\rho)\right)^2 \rho^2 d\rho = \frac{2n-2l-2+2l+1+1}{(n-l-1)!} \cdot [(n+l)!]^3$$

$n = n_r + l + 1$

$\Rightarrow n-l-1 = n_r = m$

$$= \frac{2n}{\underbrace{(n-l-1)!}_{n_r!}} [(n+l)!]^3$$

$$\Rightarrow a_{n_r+1} = 0 = \frac{n_r + l + 1 - n}{(n_r+1)[n_r + 2(l+1)]}\, a_{n_r} \qquad \text{(i)}$$

$$\Rightarrow n = n_r + l + 1 \qquad \text{iii)}$$ a tada je ispunjeno i (i)' tj. a_{n_r} ne smije biti nula jer bi tada svi bili nula za $k = 0, \dots n_r$

$n_r = 0,1,2,\dots$ $\quad l = 0,1,2,\dots$

$$\Rightarrow n = 1, 2, 3, \dots \qquad \text{Q.E.D.}$$

$l = 0, 1, 2, 3, \dots$

$n_r = 0, 1, 2, 3, \dots$ broj čvorišta valne fje. - neračunajući ono za $r = 0$ koje dolazi zbog $l+1$

$$\Rightarrow E_n = -\frac{mZ^2e^4}{2\hbar^2 n^2}$$

→ **Rezime:** Kvantni brojevi

(1) angularni orbitalni $l = 0, 1, 2, \dots (n-1)$ odreduje $M^2 = \hbar^2 l(l+1)$

(2) magnetski $m = -l, -l+1, \dots +l$ odred. proj: $M_z = \hbar \cdot m$

$\Big\}\ Y_l^m(\vartheta, \varphi)$

(3) radijalni $n_r = 0, 1, 2, \dots (n-1)$ odreduje ponaš. radijalne valne fje $R(r)$ H-atoma - broj čvorišta neračunajući ono za $r = 0$ Kad $l \neq 0$ a za $l = 0$ zadnje čvorište ne postoji

(4) glavni n - odreduje energiju

ostali se prema njemu ravnaju jer: $(n-1) = n_r + l$

$l = 0, 1, \dots n-1$

$n_r = (n-1), (n-2), \dots 0$

$$\rho = \frac{2Z}{n r_0} \cdot r \qquad r_0 = \frac{\hbar^2}{me^2}$$

$$u(r, \vartheta, \varphi) = R(r)\, Y_l^m(\vartheta, \varphi) = \frac{\vartheta_1(r)}{r} Y_l^m(\vartheta, \varphi) = C_1 \frac{\vartheta(\rho)}{r} Y_l^m(\vartheta, \varphi) = \underbrace{\frac{C_1 e^{-\frac{\rho}{2}} \cdot \rho^{l+1} L(\rho)}{r}}_{R(r)} Y_l^m(\vartheta, \varphi)$$

$$\Rightarrow u_{nlm}(r, \vartheta, \varphi)$$ valna fja.

- mogućnost visokog stupnja degeneracije za isti n tj. energiju tj. velik broj valnih fja. koje vode na istu energiju

(5) spin $\vec{s}$ $S = \frac{1}{2}, -\frac{1}{2}$ $(\hbar = 1)$ tj. spin mjerimo u jedinicama $\hbar$

(projekcija na vektor os)

→ Koliko stanja ima za n - tolika je **degeneracija**

broj m-ova za dani l

n	l	$2l+1$
	0	1
	1	3
	2	5
	⋮	
	$(n-1)$	$2n-1$

$$\sum_{n=1}^{n} (2n-1) = \frac{n}{2}[1+(2n-1)] = n^2$$

8.3.5 - isceljen broj orbitalnih kvantnih stanja

2 mogućnosti orijentacije spina

$$\Rightarrow \quad 2n^2$$

$$u_{nlm}(r,\vartheta,\varphi) = R_{nl}(r) \cdot Y_l^m(\vartheta,\varphi)$$

$$Y_l^m(\vartheta,\varphi) = \sqrt{\frac{2l+1}{4\pi}\frac{(l-|m|)!}{(l+|m|)!}}\, P_l^m(\cos\vartheta)\, e^{im\varphi}$$

čvorista za $r=0$ za $l = 1,2,3,\ldots$

$n_r = n-(l+1)$ čvorišta

$$R_{nl}(r) = -\sqrt{\left(\frac{2Z}{r_0 n}\right)^3 \frac{n_r!}{2n[(n+l)!]^3}}\, e^{-\frac{\varrho}{2}} \cdot \varrho^l \underbrace{L_{n+l}^{2l+1}(\varrho)}_{n_r}$$

$$n = n_r + l + 1 \qquad \varrho = \frac{2Z}{r_0 n}\cdot r \qquad r_0 = \frac{\hbar^2}{me^2}$$

$n_r = 0,1,2,\ldots$

$l = 0,1,2,\ldots \qquad m = \pm l, \ldots 0$

→ grafički - kako izgledaju valne fje & vjerojatnosti za neka kvantna stanja

1° osnovno stanje - stabilno Sjetimo se $P_l^0(t) = P_l(t)$ jer $P_0^0 = 1 \quad P_1^0 = t \quad P_1' = \sqrt{1-t^2}$

$n=1$ $\begin{cases} l=0 \\ m=0 \\ n_r=0 \end{cases}$ $\Rightarrow$

$$Y_0^0(\vartheta,\varphi) = \frac{1}{2\sqrt{\pi}} P_0^0(\cos\vartheta)\cdot e^{i0\varphi} = \frac{1}{2\sqrt{\pi}}$$

$$R_{10}(r) = -\sqrt{\frac{8Z^3}{r_0^3}\cdot\frac{1}{2\cdot 1}}\, e^{-\frac{Z}{r_0}r}\cdot 1\cdot \underbrace{L_1^1(\varrho)}_{=1}$$

vodik $Z=1$

$$= -2\sqrt{\frac{1}{r_0^3}}\, e^{-\frac{r}{r_0}}(-1) = \frac{2}{\sqrt{r_0^3}}\, e^{-\frac{r}{r_0}}$$

valna fja. za stanje bez momenta impulsa

$$u_{100}(r,\vartheta,\varphi) = R_{10}(r)\cdot Y_0^0(\vartheta,\varphi) = \frac{1}{\sqrt{\pi r_0^3}}\, e^{-\frac{r}{r_0}}$$

gustoća (25)

$$\int u_{100}^2(r,\vartheta,\varphi)\, d\tau = 1 \quad \Rightarrow \quad \int_0^\infty \underbrace{R_{10}^2(r)\, r^2 dr}_{dW_r} = 1 \quad \Rightarrow \quad dW_r = \frac{4}{r_0^3} e^{-\frac{2r}{r_0}} r^2 dr$$

$\varrho = |\psi|^2 = |u|^2$ gustoća vjerojatnosti.

$$\varrho = |u|^2 = \frac{1}{\pi r_0^3} e^{-\frac{2r}{r_0}} \qquad dW = \varrho\cdot d\tau = \frac{1}{\pi r_0^3} e^{-\frac{2r}{r_0}} d\tau$$

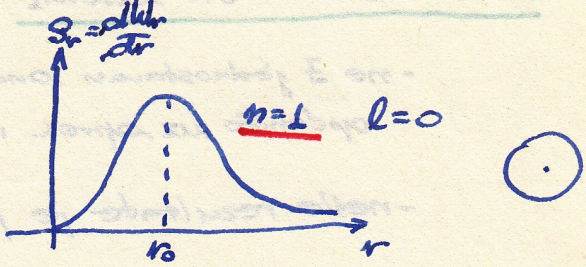
vjerojatnost da elektron u $d\tau = r^2\sin\vartheta\, dr\, d\vartheta\, d\varphi$

$$\Rightarrow dW_r = \int_0^{2\pi}\int_0^{\pi} dW = \frac{1}{\pi r_0^3} e^{-\frac{2r}{r_0}} r^2 \underbrace{\int_0^{2\pi}\int_0^{\pi} d\varphi \sin\vartheta\, d\vartheta}_{2\pi\cdot 2} \qquad (-\cos\vartheta)\Big|_0^{\pi} = 2$$

→ vjerojatnost da $\bar{e}$ nađemo u kugl. ljusci r $r+dr$

$$dW_r = \frac{4}{r_0^3} e^{-\frac{2r}{r_0}} \cdot r^2 dr$$

$$g_r = \frac{dW_r}{dr} = \frac{4}{r_0^3} e^{-\frac{2r}{r_0}} \cdot r^2$$



najvjerojatniji radijus:

$$\frac{d g_r}{dr} = 0 \Rightarrow \frac{4}{r_0}\left[2r e^{-\frac{2r}{r_0}} + r^2 \frac{-2}{r_0} e^{-\frac{2r}{r_0}}\right] = 0$$

$2r + \frac{2}{r_0} r^2 = 0 \quad 1 - \frac{r}{r_0} = 0 \Rightarrow$

$r_1 = \infty$ min
$r_2 = 0$ min
$r = r_0$ max

$$r_W = r_0 = \frac{\hbar^2}{me^2}$$

- u Bohr-ovoj teoriji: radijus gibanja elektrona

- više svjetla na Bohr-ovu teoriju kružnica r_0 dok prava strožoj kvantnoj teoriji to je najvjerojatnija udalj.

→ Komparacija s Bohr. teor.

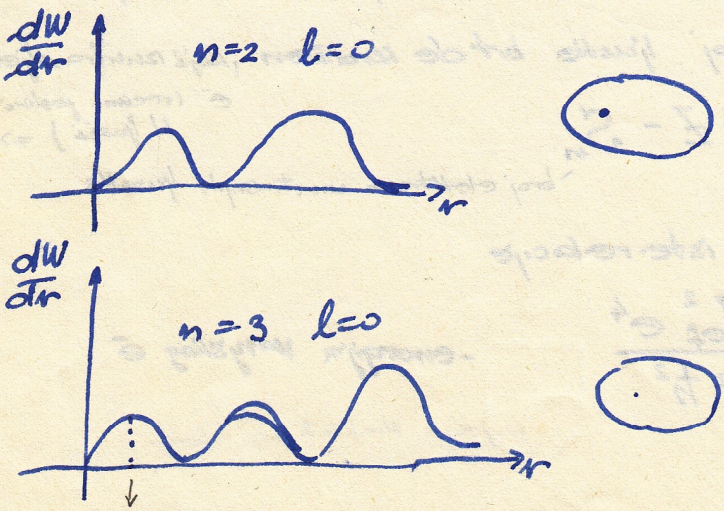
$n = n_r + n_\varphi \qquad n = n_r + l + 1$

$n_\varphi \rightarrow l+1$

$n_\varphi = n$ za $n_r = 0$

staza $\bar{e}$ kružnica → sa većim l raspodjela naboja sferna kružnica

2° $n=2$



elektron može doći do nešto manje udaljenosti i sa manjom vjerojatnosti, ali još vjerojatnije da će biti daleko od jezgre

Više elektronski atomi

- ne ∃ jednostavan analit. prilaz → egzaktan račun
  općenito uz aprox. i kompjutere
- neke rezultate je jednostavno izvući

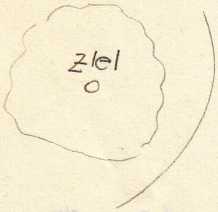
→ stanja dijelimo po glavnom kv. broju - stanja iste energije → ljuske

$2n^2$ (broj podstanja)	K	L	M	N	O
	n=1	2	3	4	5

podljuske

	s	p	d	f	g
l =	0	1	2	3	4

→ gruba aproximacija



- zbog jednostavnosti možemo zanemariti interakciju e^-
  tj. međudjelovanje ljusaka se poništava

→ dominantna interakcija e^- s jezgrom i e^- unutrašnjih ljusaka

pretp.: - unutrašnje ljuske su sferno simetr.
(mišu uslijed ind. vanjskim elektr.)
distribucija naboja
kao da je cijeli naboj unutrašnjih ljusaka smješten uz jezgru

⇒ efektivni naboj ljuske brt će izražen (koji izvana djeluje na neki e^- (recimo jedini elektron u N ljusci) ⇒ $S_n = S_K + S_L + S_M$

$$Z_{ef} = Z - S_n$$

S_n - broj elektrona unutrašnjih ljusaka

→ možemo primijeniti isto relacije

$$E_n \simeq -\frac{m Z_{ef}^2 e^4}{2 n^2 \hbar^2}$$

- energija vanjskog e^-

izvješća kvalitativna inform.

alkalijski metali → 1 valentni $\bar{e}$ → $Z_{ef} = 1$ (S_{in} = 1 $\bar{e}$ u vanj. ljusci ⇒ $(Z-1)$ u unutr. ljuskama)

⇒ E_n kao $\bar{e}$ u H-atomu zbog glavnog kvantnog broja n

nareckimo $n=1$ gdje su ostali $\bar{e}$ i koji čine K ljusku

$\omega_{mn} = \frac{E_n - E_m}{\hbar}$ u optičkom dijelu spektra za prijelaze između vanj. nivoa

→ za unutrašnja stanja visoke frekv. tj. situacija potpuno drugačija jer ako u predzadnjoj ima 9 elektrona

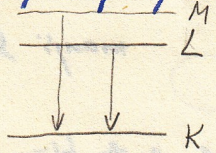
Kod prijelaza $\bar{e}$ kod unutrašnjih ljusaka

npr. $Z_{ef} = 10$ ⇒ $E \sim 10^2 \times$ veće ⇒ $\omega \sim 10^2 \times$ veće

⇒ Karakteristični Röntgenski spektri (zraka) - karakteristični za pojedini element

- ostaju konstantni pri faznim prijelazima: kom. promjenama za koje su odgovorni vanjski $\bar{e}$, a unutrašnjost se ne mijenja

→ objašnjenje Moseley-evog zakona



K_α $L \to K$

K_β $M \to K$

- bombardiranjem sa projektilima visokih energija → oslobađaju se unutrašnji (ljuske) nivoi (oslobođ. kv. stanja) na koja skaču $\bar{e}$ iz vanjskih nivoa (ljusaka)

$E_n = \frac{-m(Z-1)^2 e^4}{2n^2 \hbar^2}$

naime: K-ljuska $n=1$ $2n^2 = 2$ $\bar{e}$ od kojih je jedan izbijen

⇒ $Z_{ef} = Z - 1$ jer onaj koji je ostao kao da poništava +naboj jezgre

$K \to n=1$
$L \to n=2$
$\Big\}$ ⇒ $K_\alpha = \omega_{21} = \frac{E_2 - E_1}{\hbar} = \frac{m(Z-1)^2 e^4}{2\hbar^3}\left(-\frac{1}{4} + \frac{1}{1}\right)$

⇒ $(Z-1)^2 = a\,\omega$

⇒ $\underline{Z = 1 + \sqrt{a\,\omega}}$

Moseley-ov zakon

veza rednog broja Z i karakterist. spektra

pogledaj Sup. Mod fiz

→ objašnjenje periodnog sustava - moguće jer broj $\bar{e}$ veći od 1 ne mijenja broj kvantnih stanja, već samo oblik valnih fja.

Pauli: → u jednom kvantnom stanju može biti samo jedan $\bar{e}$

karakteriziran sa n, l, m, S

odredit će samo jednu valnu fju. $\bar{e}$ $\psi^{spin}_{nlm}(r,\vartheta,\varphi)$

$2n^2$

$n=1$

1 H
2 He
} $l=0$ $s=\frac{1}{2}$ $-\frac{1}{2}$

$n=2$ & $n=1$ $l=0$

3 Li
4 Be
} $l=0$

5 B
6 C
7 N
8 O
9 F
10 Ne
} $n=1$ $l=0$; $n=2$ $l=0$; $l=1$

$(2l+1)$ mogućnosti

$n=3$

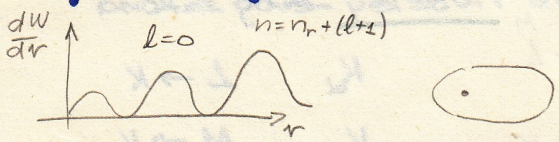
11 Na
12 Mg
} $l=0$

13 Al
14 Si
15 P
16 S
17 Cl
18 Ar
} $l=1$

proradi!!! još

$n-1, l=0$ može imati jaču energ. veze nego $n, l=n-1$

$n, l=n-1$



manji l → veća energija

⇒ 19 K $n=4$
20 Ca $l=0$

fj. ↑ vjerojatnost da dođe blizu jezgre pa ako je u tom podr. ↓ zasjenjenje ostalih $\bar{e}$ je malo

$n=3$ tek nakon toga
$l=2$

pa energija veze ovis. o angul. kv. broju

? to veća što je veći l

Ortogonalnost valnih fja.

$\hat{H} u_{n\ell m} = E_n u_{n\ell m} \;/\cdot u_m^*$ $\quad \hat{H} = -\frac{\hbar^2}{2m}\Delta + U$ - realan operator

$\hat{H}^* = \hat{H}$

1-Dim: $\Rightarrow u(x) = e^{i\varphi} u^*(x)$

$u_n(R) = 0$ R - rub područja

(?) nađene: - ∃ niz rješenja s različitim vlj. energija

$H u_m = E_m u_m$ $\quad u_m(R) = 0 \Rightarrow u_m^*(R) = 0$

$H^* = H \Rightarrow$ $\quad H u_m^* = E_m u_m^* \;/\cdot u_n$

integriramo po cijelom području

$\Rightarrow$

$$\int (u_m^* H u_n - u_n H u_m^*)\, d\tau = (E_n - E_m)\int u_m^* u_n\, d\tau$$

$u_m^* \hat{U} u_n - u_n \hat{U} u_m^* = 0.$

$$-\frac{\hbar^2}{2m}\int (u_m^* \Delta u_n - u_n \Delta u_m^*)\, d\tau = (E_n - E_m)\int u_m^* u_n\, d\tau$$

$\vec{\nabla}(u_m^* \vec{\nabla} u_n - u_n \vec{\nabla} u_m^*)$

$$-\frac{\hbar^2}{2m}\int_S (u_m^* \vec{\nabla} u_n - u_n \vec{\nabla} u_m^*)\, d\vec{f} = (E_n - E_m)\int u_m^* u_n\, d\tau$$

površ. elem.

površina, granica područja

$|d\vec{f}| \sim r^2$

$\Rightarrow (E_n - E_m)\int u_m^* u_n\, d\tau = 0$

za dobro ponašane valne fje. na rubu područja Σ zanemarujemo

- uz pretpostavku da za $R \to \infty$ pad val fja. k nuli brži nego rast površinskog elementa $\sim r^2$

$\lim_{\substack{\text{rub } R\to\infty \\ r\to\infty}} u(R)\cdot r^2 = 0$

(motivacija: H-atoma val. fja. pada exp.)

1° $E_n \neq E_m$ $\Rightarrow n \neq m$ $\quad \int u_m^* u_n\, d\tau = 0$ $\quad (i)$

2° Slučaj degeneracije: $u_{n\ell m}$ - kod H-atoma

$E_n = E_m$ $\quad u_n \neq u_m$ $\quad u_n, u_m$ zadovolj. istu Schrödingerovu. (pa ih možemo odabrati tako da budu lin. nezav. rješ.)

$\Rightarrow \alpha_1 u_n + \alpha_2 u_m$ rješ. te Schrödingerove.

α_1 & α_2 proizv.

$\mathcal{L}_1$ odred. iz (i) t. $\int \cdot = 0$

$\mathcal{L}_2$ odred. iz uvjeta normiranja

(*) pomoć: $\Rightarrow \int u_m^* u_n d\tau = 0$ kad $u_m \neq u_n$ za $E_n = E_m$

možemo ujedno reći:

$$\int u_m^* u_m d\tau = \delta_{nm} \quad \text{(ii)}$$

izražava ortogonalnost normiranih vlastitih fja. $u(\vec{r})$

$n=m \Rightarrow = 1$ $\Leftrightarrow$ Kvadrat valne fje. daje gustoću vjerojatnosti.

str (19) $H\psi = -\frac{\hbar}{i}\frac{\partial \psi}{\partial t}$ za $\frac{\partial u}{\partial t} = 0$ $\Rightarrow$ separacija $\psi(\vec{r},t) = u(\vec{r})\varphi(t)$

$$\Rightarrow \psi(\vec{r},t) = \sum_n C_n u_n(\vec{r}) e^{-\frac{i}{\hbar}E_n t}$$

iz $H\psi = -\frac{\hbar}{i}\frac{\partial \psi}{\partial t}$

- opće rješenje izgrađeno iz spektra rješenja
- $\rightarrow$ pretp. kvantiz. stanja energija E_n dokaz Sypak II 70. za 1-D im. slučaj inače bi umjesto $\sum$ bio $\int$

- odredivanje konstanti C_n

iz poč. uvjeta: $g(\vec{r}) = \psi(\vec{r},0) = \sum_n C_n u_n(\vec{r}) \quad / \cdot u_n^* \int d\tau$

pogledaj MMF

$\rightarrow$ sutle smo pretp. svojstvo potpunosti (*)

valna fja. se može razviti po svojstv. fjama, neke fiz. veličine

$$C_n = \int u_n^*(\vec{r}) \underbrace{\psi(\vec{r},0)}_{g(\vec{r})} d\tau$$

tj. dala su to sva rješenja $\Rightarrow$ tekuća $\psi(\vec{r},t)$ izgrađena pomoću njih daje $\int |\psi|^2 = 1$

- pomoću skupa fja. u_n (svojstv. stac. Schröd. jbe) možemo predočiti novu fju. - svojstvo potpunosti fja. u_n

$\Rightarrow$ ako znamo sva rješenja u_n valna fja. je potpuno odredena

Tada je:

gustoća vjerojatnosti $- g = |\psi|^2 = \sum_n \sum_m C_n^* C_m e^{i\omega_{nm}t} u_n^*(\vec{r}) u_m(\vec{r})$

oscilira s nizom Bohrovih frekvencija

$$\omega_{nm} = \frac{E_n - E_m}{\hbar}$$ Bohr-ova frekvencija

Da bi valna fja. zadovala gustoću vjerojatnosti, mora biti

$$\int |\psi|^2 d\tau = 1 \overset{\text{(ii)}}{\Rightarrow} \sum_n |C_n|^2 = 1$$

$\omega_{nn} = 0$ sigurnost

original

(*)

$$\int (\alpha_1 u_n + \alpha_2 u_m)^* (\alpha_1 u_n + \alpha_2 u_m) d\tau = 1$$

$$|\alpha_1|^2 \int u_n^* u_n d\tau + |\alpha_2|^2 \int u_m^* u_m d\tau + \alpha_2^* \alpha_1 \underbrace{\int u_m^* u_n d\tau}_{0} + \alpha_1^* \alpha_2 \int u_n^* u_m d\tau = 1$$

normir. & (i) $\Rightarrow$ $|\alpha_1|^2 + |\alpha_2|^2 = 1$

dokaz: ili zahtijevamo:

u_n, u_m, $\alpha_1 u_n + \alpha_2 u_m$ normirane za (*)

$\forall \alpha_1, \alpha_2$

odaberimo: $\alpha_1 = \frac{1}{\sqrt{2}}$ $\alpha_2 = \frac{1}{\sqrt{2}}$

(*) & (i) $\Rightarrow$ $\frac{1}{2} + \frac{1}{2} + \frac{1}{2} \int u_m^* u_n d\tau + \frac{1}{2} \int u_n^* u_m d\tau = 1$

$$\Rightarrow \int u_m^* u_n d\tau + \int u_n^* u_m d\tau = 0$$

$$\int (u_m^* u_n + u_n^* u_m) d\tau = 0 \quad \text{i)}$$

integracija po realnim varijablama

bolje $\int u_m^* u_n d\tau = -\int u_n^* u_m d\tau = -\left(\int u_m^* u_n d\tau\right)^*$

za $\forall \vec{r}$ $\Rightarrow$ $\int u_m^* u_n d\tau = a \cdot i$ $a \in R$

može $a = 0$

odaberimo: $\alpha_1 = \frac{i}{\sqrt{2}} \quad \alpha_2 = \frac{1}{\sqrt{2}} \Rightarrow \begin{matrix} \alpha_2^* \alpha_1 = \frac{i}{2} \\ \alpha_1^* \alpha_2 = -\frac{i}{2} \end{matrix}$

**) & *) $\Rightarrow \frac{1}{2} + \frac{1}{2} + \frac{i}{2}\int \mu_m^* \mu_n d\tau - \frac{i}{2}\int \mu_n^* \mu_m d\tau = 1$

$\Rightarrow \int (\mu_m^* \mu_n - \mu_n^* \mu_m) d\tau = 0$ iii)

i) & iii) $\Rightarrow$ 2hrojim $2\int \mu_m^* \mu_n d\tau = 0$

→ fiz. značenje koef. C_n

$|C_n|^2$ - vjerojatnost da se sistem nalazi u kvantnom stanju n, s vlastitom fom. u_n i energijom E_n

sumirano daje vjerojatnost ili u n ili u m

Ekvivalentnost Heisenberg-ove i Schröd. Q.M.

$$H u_n = E_n u_n \qquad p \to \frac{\hbar}{i}\frac{\partial}{\partial q}$$

sugerira da opć. proizv. fiz. veličina

$$G(q,p) \to G\left(q, \frac{\hbar}{i}\frac{\partial}{\partial q}\right) \equiv \hat{G} \quad \text{- operator}$$

$$G_{nm} \overset{\text{def.}}{=} \int u_n^* \hat{G} u_m \, d\tau \quad (i)$$

trrolimo da predstavlja elem. matrice

1° zadovoljava algebru matričnog računa

$$(G \pm F)_{nm} \overset{\text{def.(i)}}{=} \int u_n^* (\hat{G} \pm \hat{F}) u_m \, d\tau = G_{nm} \pm F_{nm}$$

$\hat{G}u_m \pm \hat{F}u_m$

$$(GF)_{nm} \overset{\text{def.(i)}}{=} \int u_n^* \hat{G}\hat{F} u_m \, d\tau = \to$$

razvijemo po potpunom skupu fja.

$$\hat{F} u_m^{(\vec{r})} = \sum_l C_l u_l^{(\vec{r})} \Rightarrow C_l = \int u_l^{*(\vec{r})} \hat{F} u_m^{(\vec{r})} d\tau \overset{(i)}{=} F_{lm}$$

$$\to = \int u_n^{*(\vec{r})} \hat{G} \sum_l F_{lm} u_l^{(\vec{r})} d\tau \overset{\text{prostp. da redoslijed integracije i sumacije možemo izmijeniti - za jednoliko konvarg. red}}{=} \sum_l F_{lm} \cdot \int u_n^{*(\vec{r})} \hat{G} u_l^{(\vec{r})} d\tau$$

$$\overset{(i)}{=} \sum_l F_{lm} \cdot G_{nl} = \sum_l G_{nl} \cdot F_{lm}$$

2° treba pokazati da iz Schröd. formulacije i ove def. matrice mora slijediti:

a) pravilo komutacije koord. i impulsa

b) Hamiltonijan je dijagonalna matrica

a) za konjugiran par $[\hat{Q}_i, \hat{p}_j] = -\frac{\hbar}{i}\delta_{ij}\cdot E$ ← jed. matrica

$i=j$ $\underline{(pQ - Qp)_{nm}} = \int u_n^*(\vec{r}) \left(\left(\frac{\hbar}{i}\frac{\partial}{\partial Q}\right) \cdot Q - Q\left(\frac{\hbar}{i}\frac{\partial}{\partial Q}\right) \right) u_m(\vec{r})\, d\tau =$

$\frac{\partial}{\partial Q}(Q u_m) = 1 u_m + Q \cdot \frac{\partial u_m(\vec{r})}{\partial Q}$ ← nazad na $[Q u_m(\vec{r})]$

$= \frac{\hbar}{i} \int u_n^*(\vec{r})\, u_m\, d\tau \overset{(ii)}{=} \underline{\frac{\hbar}{i}\delta_{nm}}$

$\Rightarrow$ dijagonalna matrica i to jedinična

a to je upravo: $[p, Q] = \frac{\hbar}{i} E$ (4) / $[p_i, Q_j] = \frac{\hbar}{i}\delta_{ij} E$ | $[p_i Q_j - Q_j p_i] \to i \neq j$

$\frac{\hbar}{i}\left[\frac{\partial}{\partial Q_i}(Q_j u_m) - Q_j \frac{\partial}{\partial Q_i}(u_m)\right]$

$= \frac{\hbar}{i}[0 \cdot u_m + 0] = 0$

Kad Q & p nebi tvorile konjug. par, tada bi te dvije veličine komutirale

→ analogno i ostale $(Q_i Q_j - Q_j Q_i)_{nm} = 0$

b) H - dijagonalna

$\underline{H_{nm}} = \int u_n^* \underbrace{\hat{H} u_m}_{\text{Schröd.} = E_m u_m} d\tau = E_m \int u_n^* u_m\, d\tau = \underline{E_m \delta_{nm}}$

- i na dijagonali su stac. stanja : (i) ishodište Heisenbergove postavke

→ potpuna ekvivalencija gornjeg i drugog pristupa

(i)

(i)

Srednje vrijednosti u Q.M.

$\psi^*\psi = g$ - u klas. fizici sr. vrij. je integrirana gustoća vjerojat. pomnož. s vrijednosti te veličine

- u Q.M. $\forall$ vel. $G(q,p)$ pridružen operator $\hat{G}$

Postulat

$$\bar{G}^{(q,p)} = \int \psi^* G^{(q,p)} \psi \, d\tau$$

- po cijelom prostoru

- opravdanost pokazuje detaljna analiza - da je ovakva def. sr. vrijednosti neke fiz. veličine razumna
- srednja vrijednost preko čistog spektra stanja

već: $G_{nm} = \int \mu_n^* \hat{G} \mu_m \, d\tau$ je davalo sr. vrijednost, ali za jedno stanje

poopćenje izračunavanja

$$\Rightarrow \quad \bar{G}^{(q,p)} = \sum_n \sum_m c_n^* c_m e^{i\omega_{nm} t} G_{nm} \qquad (iii)$$

$$\psi(\vec{r},t) = \sum_n c_n \mu_n(\vec{r}) e^{-\frac{i}{\hbar} E_n t}$$

$$\int \psi^* G \psi \, d\tau = \sum_n \sum_m c_n^* c_m \mu_n^* G \mu_m e^{i\omega_{nm} t} \, d\tau$$

izmjena realosl. $\sum\sum$ i $\int$

$$= \sum_n \sum_m c_n^* c_m e^{i\omega_{nm} t} \int \mu_n^* G \mu_m \, d\tau$$

→ Konjug. kompleks.

$$\bar{G}^{*(q,p)} = \sum_n \sum_m c_n c_m^* e^{-i\omega_{nm} t} G_{nm}^* = \text{izmjena realosl. sumacije pr. vrijedi distribucija}$$

$\omega_{nm} = -\omega_{mn}$

$$= \sum_n \sum_m c_m^* c_n e^{i\omega_{mn} t} G_{nm}^* = \sum_n \sum_m c_n^* c_m e^{i\omega_{nm} t} G_{nm}^*$$

jer je svejedno da li indeks i po kojem sumiramo pišemo n ili m

- ovdje ispitujemo realne fizičke veličine

$$\Rightarrow \bar{G}^{(q,p)} = \bar{G}^{*(q,p)} \quad \Rightarrow \quad G_{nm} = G_{mn}^*$$

Hermitske (sim.) matrice

→ fizičkim veličinama su pridružene hermitske matrice & diferencijalni operatori

Heisenberg Schröd.

→ svojstvo pridruž. dif. operatora koji def. te matrične elemente

$$\int \mu_n^*(\vec{r}) \hat{G} \mu_m(\vec{r}) \, d\tau = \int \mu_m(\vec{r}) \hat{G}^* \mu_n^*(\vec{r}) \, d\tau \quad \Rightarrow \hat{G} \text{ hermitski operator}$$

$$= \left(\int \mu_m^* \hat{G} \mu_n \, d\tau \right)^*$$

Koji def. hermi. matricu

napomena: realne fiz. velič. $\Rightarrow \hat{G} = \hat{G}^*$ i operatori su realni za $\vec{p} \to \frac{\hbar}{i} \vec{\nabla}$

→ ako za iste val. fje kojе zadovoljavaju $\hat{H}u_n = E_n u_n$

postavimo: - problem odred. svojstvenih vrijednosti operatora $\hat{G}$ čije su svojstv. (vektori) fje. u_n

$G \to \hat{G}u_n = g_n u_n$ (*) $/u_m^* \int d\tau$ - kako za njih glasi izraz za sr. vrij. i kakve matrice su pridružene tim veličina

$\Rightarrow G_{mn} = g_n \delta_{nm}$ (iv) → na dijagonali su srednje vrij.

- ako vrijed. (*) onda su veličinama G_{mn} pridruž. g_n

$\bar{G} = \sum_n \sum_m c_n^* c_m e^{i\omega_{nm}t} G_{mn}$

(iii) $\overset{\omega_{nm}=0}{\Rightarrow}$ $\bar{G}^{(s,p)} = \sum_n |C_n|^2 g_n$ - vrijednost veličine G u n-tom kvantnom stanju

vjerojatnost da sustav nađe u n-tom kv. stanju

$\Rightarrow$ poopć. $\bar{G} = \int G s \, d\phi$ kad nemam diskretnih stanja

→ za stanje $u_n^{(\vec{r})}$ $\hat{H}u_n^{(\vec{r})} = E \cdot u_n^{(\vec{r})}$ sustav se nalazi u tom stanju s energijom E

spec.: ako $\psi(\vec{r},t) = C u(\vec{r}) e^{-\frac{i}{\hbar}Et}$

$$\bar{G} = \int u_{(\vec{r})}^* \hat{G} u \, d\tau$$

↑ zbog (*) dokaz na V: 17.

$\bar{G} = \int \psi^* \hat{G} \psi \, d\tau$ ako je $\psi(\vec{r},t) = C u(\vec{r}) e^{-\frac{i}{\hbar}Et}$

→ što znači precizno mjeriti veličinu?

- neodredenost kao u statist. fizici (formalno ista def., ali s drugom def. sr. vrij.)

$$(\Delta G)^2 \overset{def.}{=} \overline{(G - \bar{G})^2} = \bar{G^2} - \bar{G}^2$$

$$\bar{G^2} = \int u_{(\vec{r})}^* \hat{G}\hat{G} u^{(\vec{r})} d\tau$$

spec. slučaj (*) → $\hat{G}$ zadovolj. jbu. svojstvenih vlast. vrij. u tom kvantnom stanju

$\hat{G}u = gu$

$$\left.\begin{aligned} \Rightarrow \bar{G} &= \int u^* \hat{G} u \, d\tau = g \int u^* u \, d\tau = g \\ \bar{G^2} &= g \int u^* \hat{G} u \, d\tau = g^2 \end{aligned}\right\} \Rightarrow (\Delta G)^2 = 0$$

$\Rightarrow$ ako operator $\hat{G}$ zadovolj. jbu. svojstv. vrij. tada g (jer općenito sr. vrij. predstavlja jedinu moguću vrijednost koju u exp. možemo dobiti) predstavlja jedinu moguću vrij. koju u exp. možemo dobiti

- ne $\exists$ neodređenost veličine G u tom kvantnom stanju

Primjer: na vježbama (Virtar 1,17)

- dvije veličine čiji pridruženi hermitski operatori $\hat{A}, \hat{B}$ ne komutiraju

$$[\hat{A}, \hat{B}] = i\hat{C} \quad \Rightarrow \quad \Delta B \cdot \Delta A \geq \frac{|\bar{C}|}{2}$$

spec. $[p, Q] = \frac{\hbar}{i} \quad \Rightarrow \quad \Delta p \cdot \Delta Q \geq \frac{\hbar}{2}$

$\rightarrow$ ali ako komutiraju $\Rightarrow$ obje se veličine mogu precizno mjeriti u danom kvantnom stanju

Angularni moment

$$\vec{M} = \vec{r} \times \vec{p} \quad \rightarrow \quad \hat{\vec{M}} = \frac{\hbar}{i}\, \vec{r} \times \vec{\nabla} \qquad p_x \rightarrow \frac{\hbar}{i}\frac{\partial}{\partial x}$$

$$\Rightarrow \quad \hat{M}_x = \frac{\hbar}{i}\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$$

$$\hat{M}_y = \frac{\hbar}{i}\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)$$

$$\hat{M}_z = \frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$$

- ako je potencijal sferno simetričan $\Rightarrow U(r) \qquad r = |\vec{r}|$

$\Rightarrow \vec{M}$ - je const. gibanja

$$u(\vec{r}) = u_{nlm}(r, \vartheta, \varphi) = R_{nl}(r)\, Y_l^m(\vartheta, \varphi)$$

$$Y_l^m(\vartheta, \varphi) = C\, e^{im\varphi}\, P_l^m(\cos\vartheta)$$

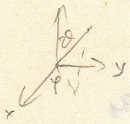
na str. 31

str. (31) → $\Delta = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\Lambda$ $\qquad \Lambda = \frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial}{\partial\vartheta}\right) + \frac{1}{\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}$

$$\Lambda Y_l^m = -l(l+1) Y_l^m \quad *)$$

svojstv. vrij. operatora Λ

→ operatore $\hat{M}_x, \hat{M}_y, \hat{M}_z$ izrazimo u polarnom sustavu



$x = r\cos\varphi\sin\vartheta$
$y = r\sin\varphi\sin\vartheta$
$z = r\cos\vartheta$

$$\frac{\partial}{\partial\varphi} = \frac{\partial x}{\partial\varphi}\frac{\partial}{\partial x} + \frac{\partial y}{\partial\varphi}\frac{\partial}{\partial y} + \underbrace{\frac{\partial z}{\partial\varphi}}_{=0}\frac{\partial}{\partial z} = -y\frac{\partial}{\partial x} + x\frac{\partial}{\partial y}$$

$$\hat{M}_z = \frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) \Rightarrow \hat{M}_z = \frac{\hbar}{i}\frac{\partial}{\partial\varphi}$$

$$\frac{\partial}{\partial\vartheta} = \frac{\partial x}{\partial\vartheta}\frac{\partial}{\partial x} + \frac{\partial y}{\partial\vartheta}\frac{\partial}{\partial y} + \frac{\partial z}{\partial\vartheta}\frac{\partial}{\partial z}$$
$$= \cos\varphi\cdot z\frac{\partial}{\partial x} + \sin\varphi\, z\frac{\partial}{\partial y} - \frac{x}{\cos\varphi}\frac{\partial}{\partial z} - \frac{y}{\sin\varphi}\frac{\partial}{\partial z} =$$

dovrši!!! na vježbama

$$\hat{M}_x = \frac{\hbar}{i}\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$$
$$\hat{M}_y = \frac{\hbar}{i}\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)$$

analogno: $\hat{M}_x = -\frac{\hbar}{i}\left(\sin\varphi\frac{\partial}{\partial\vartheta} + \cos\varphi\operatorname{ctg}\vartheta\frac{\partial}{\partial\varphi}\right)$

$$\hat{M}_y = \frac{\hbar}{i}\left(\cos\varphi\frac{\partial}{\partial\vartheta} - \sin\varphi\operatorname{ctg}\vartheta\frac{\partial}{\partial\varphi}\right)$$

$\hat{M}^2 = M_x^2 + M_y^2 + M_z^2$
$\Rightarrow \hat{M}^2 = \hat{M}_x\cdot\hat{M}_x + \hat{M}_y\cdot\hat{M}_y + \hat{M}_z\cdot\hat{M}_z$

$$\hat{\vec{M}} = \frac{\hbar}{i}\vec{r}\times\vec{\nabla} \Rightarrow \hat{M}^2 = \hat{\vec{M}}\cdot\hat{\vec{M}} = -\hbar^2(\vec{r}\times\vec{\nabla})\cdot(\vec{r}\times\vec{\nabla}) =$$
$$= -\hbar^2\left(\hat{M}_x\vec{i} + \hat{M}_y\vec{j} + \hat{M}_z\vec{k}\right)\left(\hat{M}_x\vec{i} + \hat{M}_y\vec{j} + \hat{M}_z\vec{k}\right) =$$
$$= -\hbar^2\left[\hat{M}_x\cdot\hat{M}_x + \hat{M}_y\cdot\hat{M}_y + \hat{M}_z\cdot\hat{M}_z\right] =$$
$$= -\hbar^2\Big\{\sin^2\varphi\frac{\partial^2}{\partial\vartheta^2} + \sin\varphi\cos\varphi\left(-\frac{1}{\sin^2\vartheta}\right)\frac{\partial}{\partial\varphi} + \sin\varphi\cos\varphi\operatorname{ctg}\vartheta\frac{\partial^2}{\partial\varphi\partial\vartheta}$$
$$+ \cos^2\varphi\operatorname{ctg}\vartheta\frac{\partial}{\partial\vartheta} + \cos\varphi\sin\varphi\operatorname{ctg}\vartheta\frac{\partial^2}{\partial\vartheta\partial\varphi} - \sin\varphi\cos\varphi\operatorname{ctg}\vartheta\frac{\partial}{\partial\varphi}$$
$$+ \cos^2\varphi\operatorname{ctg}^2\vartheta\frac{\partial^2}{\partial\varphi^2} + \cos^2\varphi\frac{\partial^2}{\partial\vartheta^2} - \sin\varphi\cos\varphi\left(-\frac{1}{\sin^2\vartheta}\right)\frac{\partial}{\partial\varphi}$$
$$- \sin\varphi\cos\varphi\operatorname{ctg}\vartheta\frac{\partial^2}{\partial\varphi\partial\vartheta} + \sin^2\varphi\operatorname{ctg}\vartheta\frac{\partial}{\partial\vartheta} - \sin\varphi\cos\varphi\operatorname{ctg}\vartheta\frac{\partial^2}{\partial\vartheta\partial\varphi}$$
$$+ \sin\varphi\cos\varphi\operatorname{ctg}\vartheta\frac{\partial}{\partial\varphi} + \sin^2\varphi\operatorname{ctg}^2\vartheta\frac{\partial^2}{\partial\varphi^2} + \frac{\partial^2}{\partial\varphi^2}\Big\} =$$
$$= -\hbar^2\left\{\frac{\partial^2}{\partial\vartheta^2} + \operatorname{ctg}\vartheta\frac{\partial}{\partial\vartheta} + \operatorname{ctg}^2\vartheta\frac{\partial^2}{\partial\varphi^2} + \frac{\partial^2}{\partial\varphi^2}\right\} =$$
$$= -\hbar^2\left\{\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial}{\partial\vartheta}\right) + \frac{1}{\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}\right\}$$

$\operatorname{ctg}^2\vartheta + 1 = \frac{1}{\sin^2\vartheta}$

Λ

$$\Rightarrow \hat{M}^2 = -\hbar^2\Lambda \quad (*)$$

str (11) $[M_x, M_y] = -\frac{\hbar}{i} M_z$ cikliček.

$\Rightarrow$ uz M^2 dijagonalna, samo je još jedna dijagonalna

odnosno uz $\hat{M}^2$ samo je još jedan nezavisan operator → proradi!!!

$$u_{nlm}(r,\vartheta,\varphi) = R_{nl}(r)\, Y_l^m(\vartheta,\varphi) = e^{im\varphi} \cdot \underbrace{R_{nl}(r) \cdot C\, P_l^m(\cos\vartheta)}_{Z(r,\vartheta)}$$

$$\hat{M}_z\, u_{nlm}(r,\vartheta,\varphi) = \frac{\hbar}{i}\frac{\partial}{\partial\varphi} e^{im\varphi} \cdot Z(r,\vartheta)$$

$$= \hbar m\, e^{im\varphi} Z(r,\vartheta) \qquad m = -l, -l+1, \ldots +l$$

$$= \hbar m\, u_{nlm}(r,\vartheta,\varphi) \qquad / u_{nlm}^* \int d\tau \qquad \int u_{nlm}^* u_{nlm}\, d\tau = \delta_{nnm}$$

$\hat{G} u_{nlm} = g_{nlm} u_{nlm}$
$\Rightarrow G_{nnm} = g_{nlm} \delta_{nnm}$

(iv) $\Rightarrow$ $(M_z)_{nnm} = \hbar m \cdot \delta_{nnm}$ → $\hat{M}_z$ pridružena dijagonalna matrica za $U(r)$

(*) $\Rightarrow$ $\hat{M}^2 u_{nlm}(r,\vartheta,\varphi) = -\hbar^2 \Lambda\, u(r,\vartheta,\varphi)$

$$= -\hbar^2 R_{nl}(r)\, \Lambda\, Y_l^m(\vartheta,\varphi) \qquad n = n_r + l + 1$$

$$= -\hbar^2 R_{nl}(r) [-l(l+1)] Y_l^m(\vartheta,\varphi) \qquad l = 0, 1, 2, \ldots (n-1)$$

$$= +\hbar^2 l(l+1)\, u_{nlm}(r,\vartheta,\varphi) \qquad / u_{nl'}^* \int d\tau$$

(iv) $\Rightarrow$ $(M^2)_{l'l} = \hbar^2 l(l+1)\, \delta_{l'l}$ → $\hat{M}^2$ pridružena dijagonalna matrica za $U(r)$

- dopunili smo Heisenberg. interpretaciju

jer on je samo $M_z|lm\rangle$ & $M^2|lm\rangle$

napomena: Postoji više načina da se to pokaže

a) Prilog 2 (Kompton) pokazao/i od $L_z|,m\rangle = m|,m\rangle$ $\vec{M} = \frac{e}{2m}\vec{L}$

uz L_+, L_- $\Rightarrow L^2 = l(l+1)$

b) Šupek

- Schröd. jba može se rijesiti za ograničen broj potencijala - ostalo aprox. metode

Varijacioni postupak

- jedan od onih koji omogućuje rješ. Schröd. jbe. u kompleksnijoj situaciji:

$$\hat{H}\mu_n = E_n \mu_n \quad / \cdot \mu_n^* \int d\tau$$

$$E_n = \int \mu_n^* \hat{H} \mu_n d\tau \qquad \int |\mu_n|^2 d\tau = 1$$

uvijek se pobrinemo da valna fja. bude pomnož. s faktorom da bi zadovolj. taj uvjet

→ Želimo odrediti energiju osnovnog kvantnog stanja ako ne znamo rješ. Schröd. jbe, tj. nepoznata nam je valna fja. (≈ (VI))

Pogađamo:

- probna valna fja. $\phi(\alpha, \vec{r})$ — parametar bilo kakvi npr. $e^{-\alpha \vec{r}}$ i postupamo kao da znamo valnu fju. (≈ (V))

izračunamo

$$\mathcal{E} = \int \phi^* \hat{H} \phi d\tau \qquad \int \phi^* \phi d\tau = 1$$

→ pokazuje se da je tako izračunata energija

$$\mathcal{E} \geq E_0$$

dokaz:

- razvijmo probnu fju.

$$\phi(\alpha, \vec{r}) = \sum_n a_n \mu_n(\vec{r})$$

$$\int |\phi|^2 d\tau = \sum_n \sum_m a_n^* a_m \underbrace{\int \mu_n^* \mu_m d\tau}_{\delta_{nm}} = \sum_n |a_n|^2 = 1$$

$$\mathcal{E} = \sum_n \sum_m a_n^* a_m \int \mu_n^* \underbrace{\hat{H} \mu_m}_{E_m \mu_m} d\tau = \sum_n \sum_m a_n^* a_m E_m \underbrace{\int \mu_n^* \mu_m d\tau}_{\delta_{nm}} = \sum_n |a_n|^2 E_n$$

$$\mathcal{E} - E_0 = \sum_n |a_n|^2 E_n - E_0 \sum_n |a_n|^2 = \sum_n |a_n|^2 \underbrace{(E_n - E_0)}_{\geq 0} \geq 0$$

$$\Rightarrow \quad \mathcal{E} \geq E_0$$

- mi se ovdje zaustavljamo - na ideji:

  ∃ talkoder varijaciona metoda za $E_1, E_2, \ldots$

- iz tog teorema vidimo približno odredit. energ. osnovnog stanja

  izračunamo: $\mathcal{E}(\alpha, \beta) \geq E_0$

  (α, β parametar)

  → α, β tako podesimo da $\mathcal{E}_{min}$

  $$\Rightarrow \frac{\partial \mathcal{E}}{\partial \alpha} = 0 \qquad \frac{\partial \mathcal{E}}{\partial \beta} = 0 \qquad \Rightarrow \alpha, \beta \text{ koji daju minim. vrijednost za } \mathcal{E} \rightarrow \text{najbliži } E_0!$$

- nedoumica kako odabrati probnu valnu fju. $\phi(\alpha, \beta)$

- formalizam 1 čestice proširujemo na mnoštvo čestica

  Hamiltonijan kvantnog problema

$$\hat{H} = -\frac{\hbar^2}{2} \sum_i \frac{\Delta_i}{m_i} + U$$

$$\hat{H}\psi = -\frac{\hbar}{i} \frac{\partial \psi}{\partial t}$$

stac. problem $\hat{H} u_n = E_n \cdot u_n$ za kvantizirani spektar

$$\psi(\vec{r}, t) = \sum_n C_n u_n(\vec{r})\, e^{-\frac{i}{\hbar} E_n t}$$

($\vec{r}$ | sve koordinate)

$$\int |\psi|^2 d\vec{r} = 1 \qquad *)$$

($d\vec{r}$ - elem. faznog volum.)

→ teško, nemoguće riješiti takvu fju., pogotovo ako U sadrži pot. energiju međudjelovanja

Problem jednakih čestica

- sva ista fizička obilježja (naboj) Q, m, spin, magn. moment

$\hat{H}(1,2)$ $\quad 1 \to x_1, y_1, z_1 \quad S_1$ (spin) $\quad$ dvije čestice - za više analogno

$\quad 2 \to x_2, y_2, z_2 \quad S_2$

Kvantno meh. princip - jednake čestice ne mogu razlikovati

$$\hat{H}(1,2) = \hat{H}(2,1)$$

$$\left[\hat{H}(1,2) + \frac{\hbar}{i}\frac{\partial}{\partial t}\right]\psi(1,2) = 0$$

ovisi o t, ali nam to nije važno

$|\psi(1,2)|^2$ gustoća vjerojatnosti nekih položaja čestica

zamijenimo prvu česticu s drugom

$$\left[\hat{H}(2,1) + \frac{\hbar}{i}\frac{\partial}{\partial t}\right]\psi(2,1) = 0 \qquad |\psi(2,1)|^2 \text{ -"-}$$

ekviv. čestice a na polož. 1.
b na polož. 2.

- Kada čestice zamijene mjesta → mi ih ne razlikujemo

$$\Rightarrow \quad |\psi(2,1)|^2 = |\psi(1,2)|^2$$

$$\psi(2,1) = e^{i\varphi}\cdot\psi(1,2)$$

razlikuju se samo u tom faznom faktoru

može i 2 koraka

$$\psi(1,2) = e^{i\varphi}\psi(2,1) = e^{2i\varphi}\psi(1,2)$$

$$\Rightarrow e^{2i\varphi} = 1 \quad \Rightarrow \quad 2\varphi = 2\pi n \quad \Rightarrow \quad \varphi = \pi n \quad (*) \quad \Rightarrow e^{i\varphi} = e^{in\pi} = (-1)^n = \pm 1$$

$$\Rightarrow \psi(2,1) = \pm\psi(1,2) \quad (*)$$

- valne fje. koje nastaju permutacijom dviju čestica mogu mijenjati samo predznak tj. i-tu zamij. s j-tom promjena $\pm$

- gdje u prirodi susrećemo sim., a gdje asim. valne fje.

teorija i exp.

1) Simetrična valna fja. (totalna) (u nju je uključena staza i spin)

foton, fonon, K-mezon

S = 0, 1, 2 (računati u jedinicama $\hbar$)

- opć. za sustave čestica koji se podvrgavaju Bose-Einstein-ovoj statistici:

bozoni:

2) Antisimetrična valna fja (uključuje stazu i spin) tj. ukupna valna fja ←

elektron, proton, neutron, neutrino

S = 1/2, 3/2, 5/2

- podvrgavaju se Fermi-Diracovoj statistici:

fermioni:

→ najjednostavniji slučaj - sustav bez interakcije (ili kao mala smetnja)

$$\Rightarrow U = \sum_i U_i(i)$$

$$U_{int} \approx 0 \qquad \Rightarrow \hat{H}(1,2) = \hat{H}(1) + \hat{H}(2)$$

prva čestica u stanju a opisana valnom fjom. $\psi_a(1)$

druga čestica u stanju b opisana valnom fjom $\psi_b(2)$

ukupna valna fja. je: $\psi_a(1)\psi_b(2)$ → $\hat{H}(1,2)\left[\psi_a(1)\psi_b(2)\right] + \frac{\hbar}{i}\frac{\partial}{\partial t}\left[\psi_a(1)\psi_b(2)\right] =$

(1,2) koord. 1. čestice

$= \psi_b(2)\hat{H}(1)\psi_a(1) + \psi_a(1)\hat{H}(2)\psi_b(2)$

$+ \frac{\hbar}{i}\psi_b(2)\frac{\partial\psi(1)}{\partial t} + \frac{\hbar}{i}\psi_a(1)\frac{\partial\psi(2)}{\partial t} =$

$= \psi_b(2)\left[\hat{H}(1)\psi_a(1) + \frac{\hbar}{i}\frac{\partial\psi_a(1)}{\partial t}\right] +$

$+ \psi_a(1)\underbrace{\left[\hat{H}(2)\psi_b(2) + \frac{\hbar}{i}\frac{\partial\psi_b(2)}{\partial t}\right]}_{=0} = 0$

- čestice ne razlikujemo, rješenje je i

$\psi_b(1)\psi_a(2)$

za sustav dvije čest. bez interakcije

⇒ opće rješenje je superpozicija partik. rješenja

- konst. C_1, C_2 moraju zadovolj. uvjet normiranja *) i sim. odnosno asim. ukupnog rješenja (*) (43)

uvjet sa (43)

Konst. normiranja

$$\psi(1,2) = \frac{1}{\sqrt{2}}\left[\psi_a(1)\psi_b(2) \pm \psi_a(2)\psi_b(1)\right]$$

\+ sim. fja. bozoni
− asim. fja. fermioni

- sistemom

- fermionsko asim. rješenje

$$\psi_{as}(1,2) = \frac{1}{\sqrt{2}}\begin{vmatrix} \psi_a(1) & \psi_a(2) & \psi_a(3) \\ \psi_b(1) & \psi_b(2) & \psi_b(3) \\ \psi_c(1) & \psi_c(2) & \psi_c(3) \end{vmatrix}$$

poopć.

II čest na položaju 2

→ za $\psi_a = \psi_b \Rightarrow \psi_{as}(1,2) = \begin{vmatrix} \psi_a(1) & \psi_a(2) \\ \psi_a(1) & \psi_a(2) \end{vmatrix} = 0$

$\Rightarrow \psi_a(1)\psi_a(2) - \psi_a(2)\psi_a(1)$

⇒ takvo rješenje ne ∃ za fermionske sisteme u kojem bi dva ili više fermiona bili u istom kvantnom stanju

Pauli-ev princip

→ mnošvo čestica ⇒ rješava stat. fizika

Elementi kvantne stat. fizike

- kvantizacija energ. nivoa → III z.t.d.

Harmonički oscilator (1 - II im.)

- našli smo u kvantnoj fizici $E_N = \frac{\hbar\omega}{2}(2N+1)$ i) $N = 0,1,2,\ldots$ kv. broj

- M. Planck 1900. hipoteza $E_N = N\hbar\omega$ ii) $N = 0,1,2,\ldots$

razlika - nulta točka energije H.O. je $\frac{\hbar\omega}{2}$ zbog relac. neodređ.

za razm. H.O. od intenzna kvantizacija i razmak $\hbar\omega$

$\hbar\omega$

→ H.O. na temp. T

→ zanima nas srednja mjesalnost energije na danoj temp. T

primj. Klas. statistika - Boltzmann: $\frac{N_i}{g_i} \ll 1$ pretpostavka

stanje E_N ima N kvazičestica

Kanonska raspodjela:

particiona fja. $Z = \sum_{N=0}^{\infty} e^{-\beta E_N}$ $\quad \beta = \frac{1}{kT}$

jer $Z = \sum_i g_i e^{-\beta E_i}$ faktor degeneracije $g_i = 1 \ \forall i$ (broj kvantnih stanja iste energije)

jer jedna valna fja vodi na $E_N = \frac{\hbar\omega}{2}(2N+1)$ str (28)

$\psi_n(x) = A e^{\frac{x^2}{2a^2}} H_n\left(\frac{x}{a}\right)$

? dok na $E_N = \frac{\hbar\omega}{2}(2N-1)$ $N = 1, 2, \ldots$ vodi drugu

provedi!!! da li je ista kvantka od

$$\Rightarrow Z = e^{-\beta\frac{\hbar\omega}{2}} \sum_{N=0}^{\infty} e^{-N\beta\hbar\omega}$$

$$Z = e^{-\beta\frac{\hbar\omega}{2}} \cdot \frac{1}{1 - e^{-\beta\hbar\omega}}$$

particiona fja. linearnog harm. osc.

pogledaj!!!

za 1 čestica - fj. 1 H.O.

$$\bar{E} = -\frac{d}{d\beta} \ln Z \qquad \ln Z = -\beta\frac{\hbar\omega}{2} - \ln\left(1 - e^{-\beta\hbar\omega}\right)$$

$$-\frac{d}{d\beta}\ln Z = \frac{\hbar\omega}{2} + \frac{-(-\hbar\omega)e^{-\beta\hbar\omega}}{1 - e^{-\beta\hbar\omega}} = \frac{\hbar\omega}{2} + \frac{\hbar\omega}{e^{\beta\hbar\omega} - 1}$$

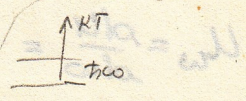
$$\bar{E} = \frac{\hbar\omega}{2} + \frac{\hbar\omega}{e^{\frac{\hbar\omega}{kT}} - 1}$$

neovisno o T $\Rightarrow$ i) $\Leftrightarrow$ ii) za 1-dim. podatke

toplinski kapacitet:

$$\frac{d\bar{E}}{dT} = K\left(\frac{\hbar\omega}{kT}\right)^2 \frac{e^{\frac{\hbar\omega}{kT}}}{\left(e^{\frac{\hbar\omega}{kT}} - 1\right)^2}$$

$$\frac{-\hbar\omega\, e^{\frac{\hbar\omega}{kT}}\left(-\frac{\hbar\omega}{kT^2}\right)}{\left(e^{\frac{\hbar\omega}{kT}} - 1\right)^2} = K\left(\frac{\hbar\omega}{kT}\right)^2 \frac{e^{\frac{\hbar\omega}{kT}}}{\left(e^{\frac{\hbar\omega}{kT}} - 1\right)^2}$$



1° $kT \gg \hbar\omega$ visoke temp. - kvantizacija se gotovo ne opaža → očekujemo klasičan rezultat

$$e^{\frac{\hbar\omega}{kT}} = 1 + \frac{\hbar\omega}{kT} + \frac{1}{2}\left(\frac{\hbar\omega}{kT}\right)^2 + \ldots$$

komparirati sa $\left(\frac{\hbar\omega}{2}\right)$

$$\frac{1}{1+x} \approx 1 - x \quad x \ll 1$$

$$\bar{E} = \frac{\hbar\omega}{2} + \frac{\hbar\omega}{\frac{\hbar\omega}{kT}\left(1 + \frac{1}{2}\frac{\hbar\omega}{kT}\right)} = \frac{\hbar\omega}{2} + \frac{kT}{\left(1 + \frac{1}{2}\frac{\hbar\omega}{2kT}\right)}$$

$$\bar{E} \approx \frac{\hbar\omega}{2} + kT\left(1 - \frac{1}{2}\frac{\hbar\omega}{kT}\right) = kT$$

$$\Rightarrow \bar{E} = kT \qquad \frac{d\bar{E}}{dT} = K$$

↑ ekviparticiona energija $\frac{kT}{2} + \frac{kT}{2}$

$$\frac{d\bar{E}}{dT} = K\left(\frac{\hbar\omega}{kT}\right)^2 \cdot \frac{1 + \frac{\hbar\omega}{kT} + \frac{1}{2}\left(\frac{\hbar\omega}{kT}\right)^2}{\left(\frac{\hbar\omega}{kT}\right)^2\left[1 + \frac{1}{2}\left(\frac{\hbar\omega}{kT}\right)\right]^2} \qquad \frac{1}{(1+x)^2} \approx 1 - 2x$$

$$\approx K \cdot \left(1 + \frac{\hbar\omega}{kT} + \frac{1}{2}\left(\frac{\hbar\omega}{kT}\right)^2\right) \cdot \left(1 - \left(\frac{\hbar\omega}{kT}\right)\right) \approx K$$

→ rezultat klasične fizike

$KT \uparrow$ ——— $\hbar\omega$ - razmak stanja

2° $KT \ll \hbar\omega$ - niske temp → kvantizacija je dominantna

termički obrok nije dovoljan za pobuđivanje

$\Rightarrow e^{\frac{\hbar\omega}{KT}} \gg 1$

→ ne može se analizirati u okviru klas. stat. fizike jer kvantizacija energ. nivoa odlučna

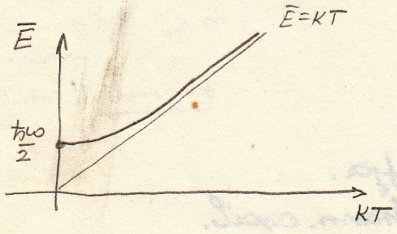
$$\bar{E} = \frac{\hbar\omega}{2} + \hbar\omega e^{-\frac{\hbar\omega}{KT}} \approx \frac{\hbar\omega}{2}$$

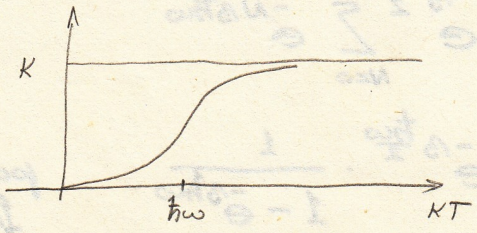
→ harm. oscilator jedva pobuđen - ostaje u najnižem stanju

daje prigušenje

$$\frac{d\bar{E}}{dt} = K\left(\frac{\hbar\omega}{KT}\right)^2 e^{-\frac{\hbar\omega}{KT}} \qquad K\hbar\omega \cdot -\frac{\hbar\omega}{K^2} \cdot -\frac{1}{T^2}$$

$T \to 0 \to 0$ III z.t.d.





→ primjena na:

Zračenje crnog tijela

→ nul energija $\frac{\hbar\omega}{2}$ irelevantna u t-dinamici

Imali smo:

$$U = 2\sum_{\vec{\varrho}} \bar{E}(\omega) \quad \bar{E}(\varrho)$$

zbog transferzalne polarizacije el.m. vala

$\vec{\varrho}$ - valni vektor

$$\to 2\cdot\int \bar{E}(\omega)\, d^3n = 2\,\frac{V}{(2\pi)^3 c^3}\int \bar{E}(\omega)\, d^3\omega$$

$$p = \frac{h}{\lambda} = \frac{h}{2\pi}\frac{2\pi}{\lambda} = \frac{h}{2\pi}\varrho \qquad \frac{2\pi}{\lambda} = \varrho_x = \frac{2\pi}{L}n_x \qquad \text{jer } e^{i\varrho_x x} = e^{i\varrho_x(x+L)}$$

$$d^3n = dn_x\, dn_y\, dn_z = \frac{L^3}{(2\pi)^3} d^3\varrho = \frac{L^3}{(2\pi)^3 c^3} d^3\omega \cdot V$$

$\omega = \varrho \cdot c \Rightarrow d^3\omega = c^3 \cdot d^3\varrho$

$d^3\omega = 4\pi\omega^2 d\omega$

$$U = \frac{V}{\pi^2 c^3}\int_0^\infty \bar{E}(\omega)\,\omega^2 d\omega = V\int_0^\infty \underbrace{\frac{1}{\pi^2 c^3}\bar{E}(\omega)\,\omega^3 d\omega}_{du}$$

$$u_\omega = \frac{du}{d\omega} = \frac{\omega^2 \bar{E}(\omega)}{\pi^2 c^3}$$

- spektralna fja. - gustoća energije na jedinicu volum. i frekvencije

$\bar{E}(\omega)$ nije isto u klas. fizici $= KT$ jer ima ekvipartic. th. za H.O.

$$\bar{E}(\omega T) = \frac{\hbar\omega}{2} + \frac{\hbar\omega}{e^{\frac{\hbar\omega}{KT}} - 1}$$

irelevantna u t-dinamici

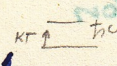
$$\Rightarrow \quad u_\omega = \frac{\hbar\omega^3}{\pi^2 c^3}\cdot\frac{1}{e^{\frac{\hbar\omega}{KT}} - 1}$$

Planck-ov zakon

1° $\hbar\omega \ll KT \Rightarrow \bar{E}(\omega) = KT$

$$\Rightarrow U_\omega = \frac{\omega^2 KT}{\pi^2 c^3}$$ → Jeans-Rayleigh

izgubio se $\hbar$ – čisto klasična formula



2° $\hbar\omega \gg KT \Rightarrow \bar{E} = \frac{\hbar\omega}{2} + \hbar\omega e^{-\frac{\hbar\omega}{KT}}$

irelevantna u termodinamici

$$U_\omega = \frac{\hbar\omega^3}{\pi^2 c^3} e^{-\frac{\hbar\omega}{KT}}$$ → Wien-ov (empirijski zakon)

$$U_\omega(T) = \frac{\hbar\omega^3}{\pi^2 c^3} \cdot \frac{1}{e^{\frac{\hbar\omega}{KT}} - 1} = \frac{T^3 k^3}{\pi^2 c^3 \hbar^2} \cdot \frac{\left(\frac{\hbar\omega}{KT}\right)^3}{e^{\frac{\hbar\omega}{KT}} - 1}$$

$$x = \frac{\hbar\omega}{KT} \qquad U_\omega(T) = C(T) \cdot \frac{x^3}{e^x - 1}$$

– tražimo max. za dani T

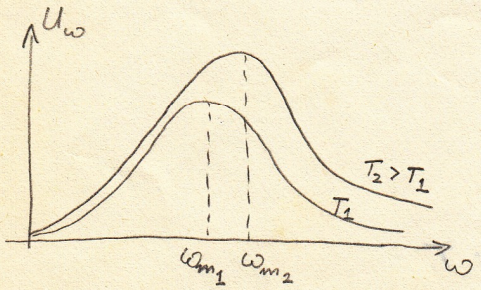
$$\frac{3x^2}{e^x - 1} + \frac{-x^3 e^x}{(e^x - 1)^2} = 0 \quad \text{za } x \neq 0 \text{ tj. } \omega \neq 0 \text{ ili } T < \infty$$

$$\frac{dU_\omega}{dx} = 0 \qquad 3x^2(e^x - 1) - x^3 e^x = 0 \quad / : x^2 \neq 0$$

$$3(e^x - 1) = x e^x$$

→ x u blizini 3 $\Rightarrow$ $x = 2{,}822 = \frac{\hbar\omega_m}{KT}$

$$\Rightarrow \omega_{max.} = \frac{2{,}822 \cdot K}{\hbar} \cdot T = 3{,}69 \cdot 10^{11} \cdot T \quad (sek^{-1})$$



→ exp. važno – kako se U_ω raspoređuje po λ

$$c = \lambda\nu = \lambda \frac{\omega}{2\pi} \Rightarrow 2\pi c = \lambda \cdot \omega \qquad \omega\, d\lambda + \lambda\, d\omega = 0 \Rightarrow \frac{d\omega}{d\lambda} = -\frac{\omega}{\lambda}$$

$$U_\lambda = \left|\frac{dU}{d\lambda}\right| \qquad \frac{d}{d\lambda} = \frac{d\omega}{d\lambda}\frac{d}{d\omega} = -\frac{\omega}{\lambda}\frac{d}{d\omega}$$

$$U_\lambda = \left|\frac{\frac{1}{\pi^2 c^3}\bar{E}(\omega)\omega^2 d\omega}{d\lambda}\right| = \frac{\omega^2 \bar{E}(\omega)}{\pi^2 c^3}\left|\frac{d\omega}{d\lambda}\right| = \frac{\omega^2 \bar{E}(\omega)}{\pi^2 c^3}\frac{\omega}{\lambda} = \frac{\omega^3 \bar{E}(\omega)}{\pi^2 c^3 \cdot \lambda} =$$

$$u_\lambda = \frac{\omega^3 \bar{E}(\omega)}{\pi^2 c^3 \lambda} \qquad 2\pi c = \lambda \cdot \omega \quad \Rightarrow \omega = \frac{2\pi c}{\lambda}$$

$$E(\omega) = \underbrace{\frac{\hbar\omega}{2}}_{\text{irelevantno}} + \frac{\hbar\omega}{e^{\frac{\hbar\omega}{kT}} - 1}$$

$$u_\lambda = \frac{(2\pi c)^3 \cdot \hbar \cdot \frac{2\pi c}{\lambda}}{\pi^3 c^3 \cdot \lambda^4} \cdot \frac{1}{e^{\frac{2\pi\hbar c}{kT\lambda}} - 1}$$

$$u_\lambda = \frac{16\pi^2 \cdot \hbar \cdot c}{\lambda^5} \cdot \frac{1}{e^{\frac{2\pi\hbar c}{kT\lambda}} - 1}$$

Planck-ov zakon

$$= \frac{k^5 \cdot T^5}{2\pi^3 \hbar^4 c^4} \cdot \frac{\left(\frac{2\pi\hbar c}{kT\lambda}\right)^5}{e^{\frac{2\pi\hbar c}{kT\lambda}} - 1}$$

$$x = \frac{2\pi\hbar c}{kT\lambda} \qquad u_\lambda = C'(T) \cdot \frac{x^5}{e^x - 1}$$

- za dani T tražimo max. od u_λ

$$\frac{5x^4}{e^x - 1} - \frac{x^5 e^x}{(e^x - 1)^2} = 0 \qquad x \neq 0 \text{ za } T, \lambda < \infty$$

$$5x^4 (e^x - 1) - x^5 e^x = 0 \quad / : x^4 \neq 0$$

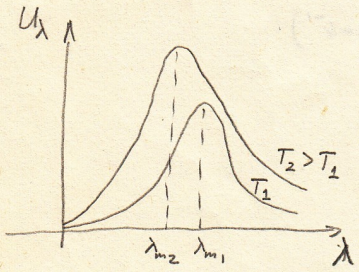
$$5(e^x - 1) = x e^x$$

- rješ. blizu 5

$$x = 4{,}965$$

$$\Rightarrow \lambda_{max} = \frac{2\pi\hbar c}{4{,}965\, kT} = \frac{0{,}29}{T} \text{ (cm)}$$

Wien-ov zakon



Ukupna energija zračenja - za dani T

$$U = \int du = V \int_0^\infty u_\omega \, d\omega$$

$$U = V \int_0^\infty u_\omega \, d\omega = \frac{V\hbar}{\pi^2 c^3} \int_0^\infty \frac{\omega^3}{e^{\frac{\hbar\omega}{kT}} - 1} d\omega = \frac{V \cdot (kT)^4}{\pi^2 (\hbar c)^3} \underbrace{\int_0^\infty \frac{x^3 dx}{e^x - 1}}_{= \frac{\pi^4}{15}}$$

preko rezidua (sing. $x = 0$)

$$x = \frac{\hbar}{kT}\omega \quad \Rightarrow d\omega = \frac{kT}{\hbar} dx$$

$$U = aV \cdot T^4 \qquad a = \frac{\pi^2 k^4}{15(\hbar c)^3}$$

Boltzmann - Stefan-ov zakon

odredena tek u Ku. stat. fiz.

toplinski kapacitet :

$$C_v = \left(\frac{\partial U}{\partial T}\right)_V = 4aVT^3$$

$T \to 0$ iščezava u skladu s III z.t.d.

entropija : $dQ = C_v dT = T dS' \Rightarrow dS' = \frac{C_v}{T} dT$

$$S' = \int_0^T \frac{C_v}{T} dT = 4aV \int_0^T T^2 dT = \frac{4}{3} aVT^3 \to 0 \text{ za } T \to 0$$

Fotonski plin

- energija H.O. za jedan H.O. $E_N = N\hbar\omega + \frac{\hbar\omega}{2}$ $N = 0, 1, 2, \ldots$

- time je opisana energija N-tog kvantnog stanja za 1. H. O.

- zračenje ćemo opisati nizom H.O.

→ Korpuskularna interpretacija

$\frac{\hbar\omega}{2}$ energija vakuumskog stanja $+ N\hbar\omega$ - sistem od N kvazi čestica, dok samo $\frac{\hbar\omega}{2}$ energija sistema kad je prazan $\hbar\omega$ - u njemu nema kvazi čestica

→ N - tumačimo kao broj fotona - .

kvazi čestica energije : $\hbar\omega$

impulsa $\hbar\vec{k}$

- U skok H.O. dajemo ili poništenje toliko fotona, koliki je skok na čestici

- el.m. zračenje : niz harmon. oscilatora određenih s ω

→ Koliki je taj broj fotona na nekoj temp. T u t.din ravn.

- na temp. T u t-din. ravnot.

$$\bar{E}(\omega) = \hbar\omega \cdot \underbrace{\frac{1}{e^{\frac{\hbar\omega}{KT}} - 1}}_{\text{- broj fotona frekv. } \omega \text{ (energije } \hbar\omega\text{) nalazi se u nekom sustavu na temp. } T}$$

$$N(\omega) = \frac{1}{e^{\frac{\hbar\omega}{KT}} - 1}$$

Planck-ova raspodjela

- **napomena!!!** možda u sebi sadrži činjenicu da u kv. fizici ne razlikujemo jednake čestice i izvedena iz kv. fizike sr. energ. $\bar{E}$ H.O.

inače $g \sim e^{-\frac{E}{KT}}$ tj. klas. raspodjela za $\hbar\omega \gg KT$

- uz fotone opisuje i fonone

- možemo naći energiju fotonskog plina, S, U, F, P

iz statist. fizike izrač. $Z \Rightarrow F \Rightarrow S = -\left(\frac{\partial F}{\partial T}\right)_V \quad P = -\left(\frac{\partial F}{\partial V}\right)_T$

→ za jedan H.O. na T → imali smo $Z = e^{-\beta\frac{\hbar\omega}{2}} \cdot \frac{1}{1 - e^{-\beta\hbar\omega}}$

uzimamo:

$$Z = \frac{1}{1 - e^{-\beta\hbar\omega}}$$

- jer faktor $e^{-\beta\frac{\hbar\omega}{2}}$ irelevantan je u t-dinamici

$$f_{(\omega)} = -KT \ln Z = KT \ln\left(1 - e^{-\beta\hbar\omega}\right)$$

- slob. energija H.O. frekv. ω

plin - sve moguće frekvencije i 2 polarizacije

$$\Rightarrow F = 2\sum_{\vec{Q}} f(\omega) = 2\sum_{\vec{Q}} KT \ln\left(1 - e^{-\beta\hbar\omega}\right)_{\nu=0}$$

- slob. energija za čitav fotonski plin

$$N_f = 2\sum_{\vec{Q}} \underbrace{N(\omega)}_{\text{broj fotona frekv. } \omega \text{ u fot. plinu}} = 2\sum_{\vec{Q}} \left(\frac{1}{e^{\frac{\hbar\omega - \nu}{KT}} - 1}\right)_{\nu=0}$$

- ukupan broj fotona

$$U = 2\sum_{\vec{Q}} \underbrace{\bar{E}(\omega)}_{\substack{\text{srednja energija fotona frekv. } \omega \\ \text{kojih ima } N(\omega) \text{ u} \\ \text{foton. plinu}}} = 2\sum_{\vec{Q}} \frac{\hbar\omega}{e^{\frac{\hbar\omega}{KT}} - 1}$$

- ukupna energija fotonskog plina

$$d^3n = \frac{L^3 V}{(2\pi)^3} d^3\vec{k} = \frac{V}{(2\pi)^3 c^3} d^3\omega \qquad \omega = k\cdot c \qquad d^3\omega = c^3 d^3\vec{k}$$

$$\sum_{\vec{k}} F(\vec{k}) \to \int F(\vec{k}) d^3n(\vec{k}) = \frac{V}{(2\pi)^3 c^3} \int F(\omega) d^3\omega = \frac{V}{2\pi^2 c^3} \int_0^\infty \omega^2 F(\omega) d\omega$$

→ (ispostavi se) $$F = kT \frac{V}{\pi^2 c^3} \int_0^\infty \omega^2 \ln\left(1 - e^{\frac{\nu - \beta\hbar\omega}{kT}}\right) d\omega \qquad \nu = 0$$

ν - uveli da bi mogli derivirati i tada ga stavimo 0

$$\left(\frac{-\frac{1}{kT} e^{\frac{\nu-\beta\hbar\omega}{kT}}}{1 - e^{\frac{\nu-\beta\hbar\omega}{kT}}}\right)_{\nu=0}$$

$$N_f = -\left(\frac{\partial \beta F}{\partial \nu}\right)_{\beta,V}$$

$$N_f = 2\sum_{\vec{k}} \frac{1}{e^{\frac{\hbar\omega}{kT}} - 1} = 2\sum_{\vec{k}} \cdot -\left(\frac{\partial \beta \frac{1}{\beta} \ln\left(1 - e^{\frac{\nu-\beta\hbar\omega}{kT}}\right)}{\partial \nu}\right)_{\beta,V}$$

$$= -\left(\frac{\partial \beta \left[kT \ln\left(1 - e^{\frac{\nu-\beta\hbar\omega}{kT}}\right)\right]_{\nu=0}}{\partial \nu}\right)_{\beta,V}$$

$$U = \left(\frac{\partial \beta F}{\partial \beta}\right)_{\nu,V}$$ - lako provjerimo

$P = -\left(\frac{\partial F}{\partial V}\right)_T$

Lako provjerimo uz: $x = \beta\hbar\omega = \frac{\hbar\omega}{kT}$

$$\omega^2 d\omega = \left(\frac{kT}{\hbar}\right)^3 dx\, x^2$$

$F \sim T^4$
$U \sim T^4$
$S \sim T^3$
$P \sim T^4$

nalazimo: $H - TS = U + PV - TS = F + PV$

$$G = F + PV = 0$$ - Gibbs-ova fja

Titranje kristalne rešetke

- Klas. teorija odstupa od exp. result. za niske temp.

1-D H.O. → particiona fja. - odbacujemo nul energiju $\frac{\hbar\omega}{2}$

$$Z = \frac{1}{1 - e^{-\beta\hbar\omega}} e^{-\frac{\beta\hbar\omega}{2}} \qquad \bar{E}_\omega = \frac{\hbar\omega}{e^{\frac{\hbar\omega}{kT}} - 1} + \frac{\hbar\omega}{2} \to N(\omega) = \frac{1}{e^{\frac{\hbar\omega}{kT}} - 1}$$

broj fonona frekv. ω

N-čestica u kristalnom sistemu → 3N ukupan broj st. slobode - oscilacionih

- u Klas. teoriji (Idio 29) pokazuje se da je ukupna energija

$$U = 3NkT$$ → na temelju tog zaključujemo da imamo 3N H.O. (Idio 29)

- ne možemo reći da ovo sistem 3N nezav. H.O., ali se može pokazati da u kvadratičnoj aprox. $E_{pot}(x_1, \ldots x_{3N})$ tako da sistem vezanih oscilatora se može zamijeniti sa ist. broj slobodnih H.O.

- pot. energiju razvijemo po malim vibracijama oko ravnotežnog položaja (I 27)
→ 3N nevezanih H.O., tj. pogodnom transformacijom

3N lin. spoj. H.O → 3N nevezanih H.O.

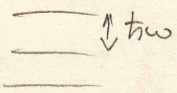
→ uvodimo analogan pojam kao kod fotona $\hbar\omega$

- gdje el. mg. sistem → kvazičestica - fotone $\hbar\omega$

Kad znamo broj fotona znamo u kojem pobuđ. stanju se nalazi sistem — uz to opisuju i širenje svjetla

∀ sloku H.O. → kvazičestica - **fonon** kvant kristalnog sistema $\hbar\omega$

niz nivoa H.O.



naziv - jer omogućuje širenje zvuka
tj. omogućuje da se kristalom šire zvučni valovi

→ slob. energija fononskog plina

$Z = \frac{1}{1-e^{\beta\hbar\omega}}$ $f(\omega) = -KT \ln Z$ slob. energija za jedan 1-dim H.O. na (44) Kod klas. kv. statist.

$$F = 3\sum_{\vec{q}} f(\omega) = 3KT \sum_{\vec{q}} \ln\left(1 - e^{\nu - \beta\hbar\omega}\right)$$ $\nu = 0$

polarizacija titranja H.O. u 3 smjera x, y, z, a nekad svjetlo u smjera x, y a širi se duž z.

→ tj. u kristalu jedan longitudinalni i dva transferzalna vala $\omega = f(\vec{q})$ inače svjetlo $\omega = c \cdot q$

- nemoraju imati isti ω, ali uzimamo neku srednju frekv. - aprox.

→ 3 moguće polarizacije

- dok kod svjetlosti obje polarizacije imaju sigurno istu frekvenciju

$$N_f = 3\sum_{\vec{q}} N(\omega) = 3\sum_{\vec{q}} \frac{1}{e^{\frac{\hbar\omega}{KT}} - 1} = -\left(\frac{\partial \beta F}{\partial \nu}\right)_{\beta, V}$$

$N(\omega)$ broj fonona u stanju frekv. ω tj. lin. H.O. frekv. ω

- ukupan broj fonona u plinu

$$U = \left(\frac{\partial \beta F}{\partial \beta}\right)_V \qquad C_V = \left(\frac{\partial U}{\partial T}\right)_V$$

$$S = -\left(\frac{\partial F}{\partial T}\right)_V$$

→ relacija za F sadrži fizički model (sva fizika), a ostalo slijedi.

↳ razvoj po prvim članovima amplituda

- iz mikroskop. proučavanja metodom statist. fizike izrač. sumu stanja i dobiv. F

- već tu sadržano koliko čemo aprox. stvarnost

→ sklad s III z.t.d. (Nernst-ovim teoremom) dolazi zbog kvantiz. energije H.O.

- u klas. fizici - nesklad zbog pretp. da jednu čestičnu možemo razlikovati.

→ **problem svodenja** $\sum_{\vec{k}} \rightarrow \int d\omega$

- dva modela koja su odigrala historijsku ulogu

1° Einstein (1907)

- pretp. da svi H.O. u kristalu titraju istom frekv., tj: ω neovisna o $\vec{k}$, dok kod svjetlosti $\omega = c\,k$

- iz očuvanja broja st. sloboda $\Rightarrow$ 3N lin. H.O.

$$\Rightarrow \quad F = 3NkT \ln\left(1 - e^{\nu - \beta\hbar\omega}\right)_{\nu=0}$$

$$U = 3N \underbrace{\frac{\hbar\omega}{e^{\beta\hbar\omega} - 1}}_{= \bar{E}(\omega)}$$

$$C_v = 3Nk \left(\frac{\hbar\omega}{kT}\right)^2 \frac{e^{\frac{\hbar\omega}{kT}}}{\left(e^{\frac{\hbar\omega}{kT}} - 1\right)^2} \xrightarrow{T \to 0} 0$$

$$S = 3Nk \left[\frac{\frac{\hbar\omega}{kT}}{e^{\frac{\hbar\omega}{kT}} - 1} - \ln\left(1 - e^{-\frac{\hbar\omega}{kT}}\right) \right] \xrightarrow{T \to 0} 0$$

$$N_f = 3N \underbrace{\frac{1}{e^{\frac{\hbar\omega}{kT}} - 1}}_{\text{broj fonona koji pripada jednom H.O. frekv. } \omega}$$

a) $kT \gg \hbar\omega$ → klas. rezultati

$$U = 3NkT \qquad \text{jer } \bar{E}(\omega) \to kT \text{ iz razvoja tj. exp. } e^{\frac{\hbar\omega}{kT}} \approx 1 + \frac{\hbar\omega}{kT}$$

$$C_v = 3Nk \qquad \text{- Dulong - Petit}$$

$$S = 3Nk \left[1 + \ln \frac{kT}{\hbar\omega} \right]$$

} Klas. rez. koji ne zadov. III z.t.d.

b) $kT \ll \hbar\omega$ niske temp.

$$U = 3N\hbar\omega\, e^{-\frac{\hbar\omega}{kT}}$$

$$C_v = 3Nk \left(\frac{\hbar\omega}{kT}\right)^2 e^{-\frac{\hbar\omega}{kT}}$$

$$S = 3Nk \left(\frac{\hbar\omega}{kT} + 1\right) e^{-\frac{\hbar\omega}{kT}}$$

} sklad sa III z.t.d. jer H.O. ostaju nepobuđeni

- eksperim. toplinski kapacitet u blizini apsol. nule pada s T^3, a ne exp.

2° Debye (1912)

- umjesto jednostavne Einst. pretp. da je ista frekv. ω za sve valne vektore uzima da ω H.O. različite ali ovise o $\vec{q}$

$$\omega = u \cdot q$$

(u – brzina prostiranja zvučnih valova)

(odgovara $\omega = c \cdot q$)

- to je tek prvi član u razvoju ω po valnom vektoru, i mijenja za jako mali q ($q^2 \to 0$)

jer $\omega = \sum_{n=0}^{\infty} a_n q^n = a_0 + a_1 q + a_2 q^2 + \dots$

$q = \frac{2\pi}{\lambda}$ → za veliki λ kristal se ponaša kao klasični kontinuum tj. kristalna struktura od malog značaja

- kao da imamo elast. sredstvo

(kao svjetlost po elast. kontinuumu)

→ na kojim T je aprox. najbolja (optimalna)

$$\mathcal{N}(\omega) = N(q) = \frac{1}{e^{\frac{\hbar\omega}{kT}} - 1}$$

- praktički doprinos $\exists$ kod. H.O. koji $\hbar\omega \lesssim kT$ *)

- međutim aprox. najbolja za $\hbar\omega \gtrsim kT$ *)', jer tada H.O. nije uopće pobuđen → kod niskih T ω pobuđen samo niskofrekv. dio spektra *)

tj. mali q

*) i *)' su kontra zahtjevi (?) $\Rightarrow \exists\, \omega_m$ za koju je aprox. najbolja odnosno $\exists$ takav T *)

→ značenje $\omega = u \cdot q \Rightarrow d^3\omega = u^3 d^3q$

kao u slučaju (svjetlosti) elektr. valova gdje $0 < \omega < \infty$

$$\sum_{\vec{q}} \to \frac{V}{2\pi^2 u^3} \int_0^{\omega_m} \omega^2 \, d\omega$$

- ograničen broj st. slobode zbog *)

$\Rightarrow q$ prima samo određ. energije

$\Rightarrow \exists$ gornja frekv. ω_m

ω_m - nalazimo iz uvjeta

per $\sum_{\vec{q}} \to \int d^3n$

$$\sum_{\vec{q}} = N \quad \text{broj atoma}$$

(neuzimajući polariz. faktor) per tada bi trebalo pisati $3N$

$$N = \frac{V}{2\pi^2 u^3} \int_0^{\omega_m} \omega^2 \, d\omega = \frac{V}{2\pi^2 u^3} \frac{\omega_m^3}{3} = \frac{V \omega_m^3}{6\pi^2 u^3}$$

$$\Rightarrow \exists\, q_{max} = \frac{\omega_m}{\mu} = \sqrt[3]{\frac{N}{V}\cdot 6\pi^2}$$

$$q_{max} = \frac{2\pi}{\lambda_{min}}$$

$$\lambda_{min} = \frac{2\pi}{q_{max}} = \sqrt[3]{\frac{V}{N}\cdot\frac{8\pi}{6}} \approx \sqrt[3]{\frac{V}{N}}$$

- reda veličine razmaka između čestica susjednih

$$F = 3KT \sum_{\vec{q}} \ln\left(1 - e^{\nu - \beta\hbar\omega}\right)_{\nu=0} = 3KT \cdot \frac{V}{2\pi^2\mu^3} \int_0^{\omega_m} \omega^2 \ln\left(1 - e^{\nu-\beta\hbar\omega}\right)_{\nu=0} d\omega$$

*) $\Rightarrow$ $K\vartheta = \hbar\omega_m$ Debye-eva temperatura

$$\Rightarrow \beta\hbar = \frac{1}{KT}\hbar = \frac{1}{T}\cdot\frac{\vartheta}{\omega_m}$$

$$x = \beta\hbar\omega \quad \Rightarrow \omega_m \Rightarrow x = \beta\hbar\omega_m = \frac{1}{KT}\hbar\omega_m = \frac{\vartheta}{T}$$

$$\frac{1}{\beta\hbar} = T\cdot\frac{\omega_m}{\vartheta}$$

$$= 3KT\,\frac{V}{2\pi^2\mu^3}\left(\frac{1}{\beta\hbar}\right)^3 \int_0^{\vartheta/T} x^2 \ln\left(1 - e^{\nu-x}\right)_{\nu=0} dx$$

$$\left(\frac{1}{\beta\hbar}\right)^3 = T^3\cdot\frac{1}{\vartheta^3}\cdot\frac{N}{V}\cdot 6\pi^2\mu^3$$

$$= 3KT\,\frac{V}{2\pi^2\mu^3}\cdot\frac{T^3}{\vartheta^3}\cdot\frac{N}{V}\,6\pi^2\mu^3 \int$$

$$= 9NKT\left(\frac{T}{\vartheta}\right)^3$$

$$F = 9NKT\cdot\left(\frac{T}{\vartheta}\right)^3 \int_0^{\vartheta/T} x^2 \ln\left(1 - e^{\nu-x}\right)_{\nu=0} dx$$

a) $T \gg \vartheta$ tako zvan. visoke temp.

$x = \frac{\hbar\omega}{KT} \Rightarrow x < 1$

zapravo $1 - e^{-x} \approx 1 - (1 - x + x^2 \ldots) \approx x$

$1 - e^{\nu-x} \approx x - \nu$

$$F = 9NKT\left(\frac{T}{\vartheta}\right)^3 \int_0^{\vartheta/T} x^2 \ln(x-\nu)\, dx$$

$$F = 3NKT\cdot\left(\ln\frac{\vartheta}{T} - \frac{1}{3}\right)$$

$$N_f = -\left(\frac{\partial\Omega F}{\partial\nu}\right)_{\beta,V} = -9N\cdot\left(\frac{T}{\vartheta}\right)^3\cdot\left(-\frac{x^2}{2}\right)_{x=\frac{\vartheta}{T}}$$

$$N_f = \frac{9}{2}N\frac{T}{\vartheta}$$

$$U = \left(\frac{\partial\beta F}{\partial\beta}\right)_V$$

$$U = 3NKT$$

$$= 3N\cdot(KT^2)\frac{\partial}{\partial T}\cdot\frac{-\vartheta}{T^2}$$

$$= -3NKT^2\cdot\frac{\vartheta}{T^2}$$

$$C_V = 3NK$$

$$S = -\left(\frac{\partial F}{\partial T}\right)_V$$

$$S = 3NK\left(\ln\frac{T}{\vartheta} + \frac{4}{3}\right)$$

$$-3NK\left[\ln\frac{\vartheta}{T} - \frac{1}{2}\right] + T\cdot\frac{T}{\vartheta}\cdot\frac{-\vartheta}{T^2}$$

} slaganje s klas. teorijom

ustvari *) $KT \leq \hbar\omega \leq K\vartheta$ - aprox. je najbolja za

? $\Rightarrow$ nije sasvim korektno

$x - \nu = \mu \quad x = \mu + \nu \quad x^2 = \mu^2 + 2\mu\nu + \nu^2$

$$\int \mu^2 \ln\mu\, d\mu + 2\nu\int \mu\ln\mu\, d\mu + \nu^2\int \ln\mu\, d\mu =$$

$$\mu^3\left[\frac{\ln\mu}{3} - \frac{1}{9}\right] + 2\nu\,\mu^2\left[\frac{\ln\mu}{2} - \frac{1}{4}\right] + \nu^2(\mu\ln\mu - \mu)$$

$$\ln\mu\left[\frac{\mu^3}{3} + \nu\mu^2 + \nu^2\mu\right] - \frac{\mu^3}{9} - \frac{\nu\mu^2}{2} - \nu^2\mu =$$

$$\frac{1}{3}\ln\mu\left[\mu^3 + 3\nu\mu^2 + 3\nu^2\mu\right] - \frac{1}{18}\left[2\mu^3 + 9\nu\mu^2 + 18\nu^2\mu\right]$$

$$\frac{\partial}{\partial\nu}\left(\frac{1}{3}(x^3 - \nu^3)\ln(x-\nu) - \frac{1}{18}(2x^3 + 3x^2\nu + 6x\nu^2 - 11\nu^3)\right)$$

$\nu = 0 \Rightarrow \frac{1}{3}x^3\ln x - \frac{x^3}{9}$

$$-2\nu^2\ln(x-\nu) + \frac{1}{3}(x^3 - \nu^3)\cdot\frac{-1}{x-\nu} - \frac{1}{18}\cdot 3x^2 - \frac{1}{3}x\nu \ldots$$

$\nu = 0 \Rightarrow -\frac{1}{3}x^3\cdot\frac{1}{x} - \frac{x^2}{6} = -\frac{x^2}{2}$

- def. niske temp.

b) $\vartheta \gg T$ tako da $\frac{\vartheta}{T} \to \infty$

Konkretno: jer aprox. najbolja za $KT \leq \hbar\omega \leq K\vartheta$

- dobiv. ist. integral kao kod zmč. el.m. valova - poopćeno za $U \sim \int_0^\infty \frac{x^3 dx}{e^x - 1} = \frac{\pi^4}{15}$

Vježbe 35.

$$N_f = 18 N \zeta(3) \left(\frac{T}{\vartheta}\right)^3$$

Riemann-ova ζ fja $\quad \zeta(k) = \sum_{n=1}^{\infty} \frac{1}{n^k}$

$$\zeta(3) = \sum_{n=1}^{\infty} \frac{1}{n^3} = 1{,}202$$

$$\zeta(4) = \sum_{n=1}^{\infty} \frac{1}{n^4} = \frac{\pi^4}{90}$$

$$F = 18 N \zeta(4) KT \left(\frac{T}{\vartheta}\right)^3$$

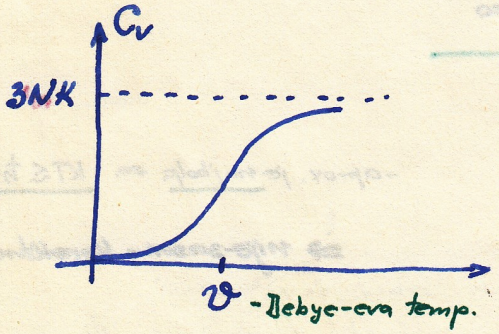
$$U = \frac{3\pi^4 NKT}{5} \left(\frac{T}{\vartheta}\right)^3$$

$$C_V = \frac{12\pi^4 NK}{5} \left(\frac{T}{\vartheta}\right)^3$$

$$S = \frac{4\pi^4 NK}{5} \left(\frac{T}{\vartheta}\right)^3$$

$\Rightarrow$ exp. potvrđeno

- sve ove ovisnosti sa T^3 imali smo i za fotone str (48)



- na sobnoj $C_V \approx 6$ cal/°K ili niži - ovisno kolika je ϑ

	Ag	Au	Be	Cu	dijamant
ϑ (°K)	215	170	1000	315	1860

$$\vartheta = \frac{\hbar}{K}\omega_m = \frac{\hbar}{K} \cdot u \sqrt[3]{\frac{N}{V} 6\pi^2}$$

brzina prostir. zvučnih valova

$\rightarrow$ za dijamant očito odstupanja od Dulong-Petit 6 cal/st. jer smo kod sobne temp. daleko u području gdje dominira T^3 tj. u donjem dijelu krivulje.

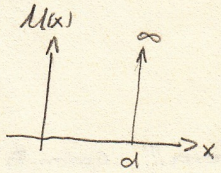
Dvoatomna molekula

- mase atoma m_1, m_2
- rezultati će strože vrijediti za različite atome, jer inače dolazi finoće zbog kv. meh. spina

→ teorija koja na niskim temp. daje izčezavanje topl. kapaciteta od rotacionih stupnjeva slobode i koja daje klas. limes

→ stupnjevi slobode - koji su kvantizirani:

translacioni - giba se u kocki brida d



u pot. jami: $U(x) = \begin{cases} \infty & x<0 \\ 0 & 0<x<d \\ \infty & x>d \end{cases}$

x,y,z osi

str (24) $\Rightarrow$ $E_1+E_2+E_3 = E = \dfrac{\hbar^2\pi^2}{2(m_1+m_2)d^2}(n_1^2+n_2^2+n_3^2)$

$d = 1\,\text{cm}$ $\quad m_1+m_2 \approx 3\cdot 10^{-24}\,\text{g}$ $\Rightarrow$

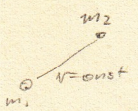
razmak između susjednih dva nivoa → $T = \dfrac{\Delta E}{K} \approx 10^{-14}$ → ? Ntrnst-ov zakon za

- to je temp. koja bi mjerila pad veličine $\frac{E}{\text{izmeđ. dva nivoa}}$

→ translac. energ. nivoi vrlo gusti.

rotacioni - energija rotatora $\quad E = U(r) + \underbrace{\dfrac{\hbar^2 l(l+1)}{2mr^2}}_{E_{rot.}}$ - centrif. potencijal

$$E_{rot.} = \frac{M^2}{2J} = \frac{\hbar^2 l(l+1)}{2J} \qquad l = 0,1,2,\ldots$$



općenito: $E_{rot} = \frac{1}{2}\sum_{k=1}^{3}\frac{\Pi_k^2}{I_k} = \frac{1}{2}\sum_{i=1}^{3} I_i\omega_i^2$ ← moment impulsa

u sustavu slob. osi: $\Pi' = \begin{pmatrix} I_1 & 0 & 0 \\ 0 & I_2 & 0 \\ 0 & 0 & I_3 \end{pmatrix}\begin{pmatrix} \omega_1 \\ \omega_2 \\ \omega_3 \end{pmatrix} \Rightarrow \Pi_i = \omega_i I_i$

$\Rightarrow T = \dfrac{\Delta E}{K} = 150$

vibracioni

$$E_n = \frac{\hbar\omega}{2}(2n+1) \qquad n = 0,1,2,\ldots \qquad T \sim 6000\,\text{K}$$

$\frac{\Delta E}{K}$

2-A molekula H_2

elektronski

$$E_n = -\frac{me^4}{2\hbar^2 n^2} \qquad n = 1,2,\ldots \qquad T \sim 150\,000\,\text{K}$$

$\frac{\Delta E}{K}$ za 1eV toliko

→ na sobnoj temp. 300 K mogu se pobuditi samo translac. i rotacioni st. slobode - pomoću termičkog gibanja

pobuđenje pri toj temperaturi

za temp. manje od sobne

translacija

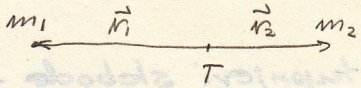
$$\bar{E}_t = \frac{3}{2}kT$$ jedne molekule, jer kvantni nivoi gusti

- trebalo bi još uvjeti formalno o nemogućnosti razlučivanja istih čestica

rotacija

$$E_l = \frac{\hbar^2 l(l+1)}{2J}$$ $M^2 = \Gamma^2$

moment inercije s obzirom na os koja je okomita na os molekule a prolazi težištem



$J = m_1 r_1^2 + m_2 r_2^2$ $\quad \vec{r} = \vec{r}_1 - \vec{r}_2$

$m_1 \vec{r}_1 + m_2 \vec{r}_2 = 0$

$\Rightarrow J = \mu r^2 = J_1$

napomena!!! Općenito bi bila rotacija oko 3 osi u T ali ne ubrajamo pod rotacijom rotaciju oko spojnice

(?) proradi: Landau (110) $I_1 = I_2 = \frac{m_1 + m_2}{m_1 + m_2} r^2$

rotator • — • ← točke nemaju masu $\Rightarrow I_3 = 0$

za sustav s(ob.os.(x_1, y_1, z_1) $I_3 = 0$

$\Gamma_i = I_i \omega_i$ $\quad I_{rot} = \frac{1}{2}(I_1\omega_1^2 + I_2\omega_2^2) \overset{I_1=I_2}{=} \frac{1}{2} I_1 (\omega_1^2 + \omega_2^2)$

$\Gamma^2 = \sum_{i=1}^{3} \Gamma_i^2 \overset{I_3=0}{=} (I_1^2\omega_1^2 + I_2^2\omega_2^2) \overset{I_1=I_2}{=} I_1^2 (\omega_1^2 + \omega_2^2)$

$E_{rot} = \frac{1}{2} I_1 \cdot \frac{\Gamma^2}{I_1^2} = \frac{1}{2}\frac{\Gamma^2}{I_1}$

- standardno računanje doprinosa

$$Z = \sum_i g_i e^{-\frac{E_i}{kT}}$$

g_i ← statist. faktor degeneracije

Koliki je g_l - tj. koliko kv. stanja ima istu energiju E_l

- teorija angul. momenta

$M^2_{nl} = \hbar^2 l(l+1)\delta_{nl}$ $\quad$ $2l+1$ vrij. za M_z

$M_{z\,mm} = m\hbar\,\delta_{mm}$ $\quad m = -l, -l+1, \ldots l$

odredi. različ. kvantna stanja - jer mijenjajući M_z ne mij. energiju

$\Rightarrow g_l = (2l+1)$

$$Z = \sum_{l=0}^{\infty} (2l+1) e^{-\frac{\vartheta_r}{T} l(l+1)}$$

$$\vartheta_r = \frac{\hbar^2}{2Jk}$$

- definirana karakteristična temp. za rotaciju

- promatramo H-atom $J = 10^{-24} \cdot (10^{-8})^2 \approx 10^{-40}\,gcm^2$

$J_{H_2} = 4{,}71 \cdot 10^{-41}\,gcm^2 \Rightarrow \vartheta_{r\,H_2} = 85{,}4\,K$

$F = N \cdot f \qquad f = -KT \ln z$ za 1 molek.

$$F = -NKT \ln z$$

(jedne molekule)

a) $T \gg \vartheta_r$ - definira visoke temp.

$\frac{\vartheta_r}{T} \ll 1$ } $\Rightarrow$ promjena l za 1 daje gotovo kontinuirano mijenjanje x_l

$$x_l = \frac{\vartheta_r}{T} l(l+1)$$

$\rightarrow$ iako $l = 0, 1, 2, 3, \ldots$ zbog $\frac{\vartheta_r}{T} \ll 1$ i kontinuir promjene x_l možemo misliti da je l i polovica $(l+\frac{3}{2} - l+\frac{1}{2})$

$$\Delta x_l = x_{l+\frac{1}{2}} - x_{l-\frac{1}{2}} = \frac{\vartheta_r}{T}\left[(l+\tfrac{1}{2})(l+\tfrac{3}{2}) - (l-\tfrac{1}{2})(l+\tfrac{1}{2})\right] = \frac{\vartheta_r}{T}(l+\tfrac{1}{2}) \cdot 2$$

$$= \frac{\vartheta_r}{T}(2l+1)$$

$$\Rightarrow z = \sum_{l=0}^{\infty} (2l+1) e^{-\frac{\vartheta_r}{T} l(l+1)} \rightarrow \sum_{x_l=0}^{\infty} \frac{T}{\vartheta_r} \cdot \Delta x_l \cdot e^{-x_l} \xrightarrow{\frac{T}{\vartheta_r} \gg 1} \frac{T}{\vartheta_r} \int_0^{\infty} e^{-x} dx = \frac{T}{\vartheta_r}$$

$\int_0^{\infty} e^{-x} dx = -e^{-x}\Big|_0^{\infty}$

$$\Rightarrow F = -NKT \ln \frac{T}{\vartheta_r}$$

$$U = \left(\frac{\partial \beta F}{\partial \beta}\right)_V = \frac{\partial}{\partial \beta}\left(-N \ln \frac{T}{\vartheta_r}\right)_V = NKT^2 \frac{d}{dT} \ln \frac{T}{\vartheta_r} = NKT^2 \frac{\frac{1}{\vartheta_r}}{\frac{T}{\vartheta_r}}$$

$$= NKT$$

$$\Rightarrow C_V^{rot} = NK$$ - u skladu s klas. teorijom i ekvipartijom

Landau $\rightarrow$ (110) za općenito atome za praven (nekolinst. vala) imaju samo dva rotac. st. slob. $\Rightarrow 2 \cdot \frac{KT}{2} = KT$

b) $T \ll \vartheta_r$ - definirano niske temp.

$\frac{\vartheta_r}{T} \gg 1$

$$\Rightarrow z = e^0 + 3 \cdot e^{-2\frac{\vartheta_r}{T}} + 5 \cdot e^{-6\frac{\vartheta_r}{T}} + 7 e^{-12\frac{\vartheta_r}{T}} + \ldots$$

! ..... $\frac{\vartheta_r}{T} \gg 1 \Rightarrow e^{-2\frac{\vartheta_r}{T}} = \frac{1}{e^{2\frac{\vartheta_r}{T}}} \ll 1 \Rightarrow e^{-6\frac{\vartheta_r}{T}} = \left(e^{-2\frac{\vartheta_r}{T}}\right)^3 \ll\ll 1$

ograničimo se $l=0$ $l=1$

$\ln(1+x) \overset{x \ll 1}{\approx} x - \frac{x^2}{2} + \frac{x^3}{3}$

$$\Rightarrow \ln z \approx 3e^{-2\frac{\vartheta_r}{T}} \Rightarrow F = -3NKT e^{-2\frac{\vartheta_r}{T}}$$

$\frac{\partial}{\partial \beta} = -KT^2 \frac{\partial}{\partial T}$

$-3N \cdot (-KT^2) \cdot -2\vartheta_r \frac{1}{T^2}$

$$U = 6NK\vartheta_r e^{-2\frac{\vartheta_r}{T}} \qquad C_V = 12NK\left(\frac{\vartheta_r}{T}\right)^2 e^{-2\frac{\vartheta_r}{T}} \xrightarrow{T \to 0} 0$$ - u skladu s III z.t.d.

$\left(\frac{\partial F}{\partial T}\right)_V = 3NK \cdot e^{-2\frac{\vartheta_r}{T}} + 3NKT \cdot \frac{+2\vartheta_r}{T^2} e^{-2\frac{\vartheta_r}{T}}$

$$S = 3NK\left(2\frac{\vartheta_r}{T} + 1\right) e^{-2\frac{\vartheta_r}{T}} \xrightarrow{T \to 0} 0$$

Vrijednosti :

	H_2	HD	D_2	HCl	Br_2	J_2
ϑ_r (°K)	85,4	64	43	15,2	0,12	0,05

$\vartheta_r \sim \frac{1}{I}$ pad s masom

ispod tzv. točke prijelaza u tekuće stanje

→ temp. iznad sobne, gdje su aktivirani vibrac. st. slobode

$\hbar\omega$ ↕

$\vartheta_{osc} = \frac{\hbar\omega}{K}$ – frekv. titranja dva atoma duž spojnice
– analogno kao kod Debye-ove temp.

	H_2	OH	NH	CH	Cl_2	J_2	K_2
$\vartheta_{osc.}$ (K)	6100	5360	4400	4100	810	310	140

za $T \approx \vartheta_{osc.}$ pobuđuju se vibrac. st. slobode – skok u topl. kapacitetu
→ porast C_v

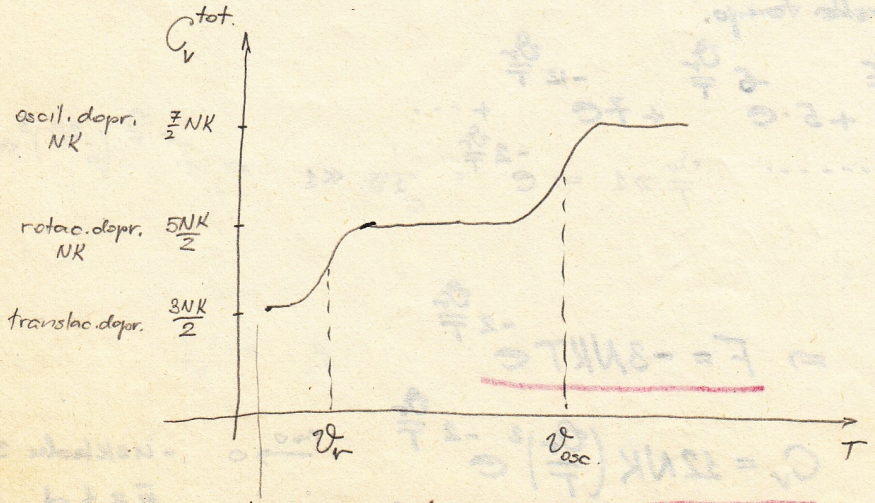
– za male oscil. aprox → H. O.

iz Einstein-ovog modela za kristalnu rešetku

a) $T \gg \vartheta_{osc.}$ $\quad KT \gg K\vartheta_{osc} = \hbar\omega$ $\quad \Rightarrow C_v^{osc.} = NK$

razlika jer ovdje umjesto 3N st. slobode ima N st. slobode

b) $T \ll \vartheta_{osc.}$ $\quad KT \ll K\vartheta_{osc} = \hbar\omega$ $\quad \Rightarrow C_v^{osc} = NK \left(\frac{\vartheta_{osc.}}{T}\right)^2 e^{-\frac{\vartheta_{osc.}}{T}}$



$\vartheta_{osc} \gg \vartheta_{rot.}$

drugačije se ponaša u blizini apsol. nule
za translac. st. slobode

Kvantna statistička fizika

- izgradnja kvantne statistike koja polazi od pretp. da jednake čestice ne razlikujemo - iz Heis. relacija neodredenosti: $\Delta q \cdot \Delta p \simeq \hbar$ u faznom prostoru

(Gibbs-ov paradox) razlikovali smo čestice

Bose - Einstein

1924 fotonski plin

1925 primjena na obične čestice

čestice cijepa je ukupna valna fja. je simetrična

$S = 0, 1, 2, \ldots$

Fermi - Dirac

1926. 1926.

ugradnja Pauli-jev princip (1925)

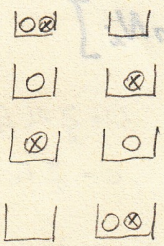
valna fja. je antisimetrična

$S = 1/2, 3/2$

Primjer:

„crna" i „bijela" kuglica stavljamo u dvije kutije → mogućnosti

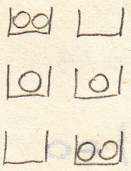
Klasična



4. mogući.

Kvantna ○ = ⊗

B. E.



3. mogući.

F. D.

Kvantno stanje sadržava najviše 1 česticu

1 mogući.

→ različiti zahtjevi dovode do bitno novih raspodjela!

- promatramo idealan plin bozona i fermiona
- pišemo termodin. vjerojatnost i njen max. → najvjerojatnija raspodjela uz uvjete

$$\sum_i N_i = N \quad / \cdot \alpha$$

$$\sum_i N_i E_i = U \quad / \cdot \beta$$

g_i - broj čelija na pojedinom kvantnom nivou energije E_i

Boltzman. $N_i = g_i e^{-1-\alpha} e^{-\beta E_i}$

Bozoni

$g_i \gg 1$
$N_i \gg 1$
} *) za i-ti energ. nivo

zbog primjene Stirling-ove formule

napomena!!! za sisteme s velikim brojem čestica je to i ispunjeno i javlja se za njih i opstr. st-dist. metode

Primjer: 7 ćelija 01 | 100|0000|1 | 10|00

$g_i - 1$ pregrada $\Leftrightarrow g_i$ ćelija
N_i čestica

$$B_i = \frac{(N_i + g_i - 1)!}{(g_i - 1)!\, N_i!}$$

broj mogućih raspodjela na i-tom energ. nivou

papir (MK)

→ t-dinamička vjerojatnost za čitav sistem → produkt za sve energ. nivoe

$$B = \prod_i \frac{(N_i + g_i - 1)!}{(g_i - 1)!\, N_i!}$$

$N \gg 1$
$N! = \left(\frac{N}{e}\right)^N$

$(N_i + g_i - 1)! = \left(\frac{N_i + g_i - 1}{e}\right)^{N_i + g_i - 1}$

*) ⇒

$$B = \prod_i \frac{(N_i + g_i)!}{g_i!\, N_i!}$$

$(N_i + g_i)! \approx \left(\frac{N_i + g_i}{e}\right)^{N_i + g_i}$

$g_i! = \left(\frac{g_i}{e}\right)^{g_i}$ $N_i! = \left(\frac{N_i}{e}\right)^{N_i}$

$$B = \prod_i \frac{(N_i + g_i)^{N_i + g_i}}{g_i^{g_i} N_i^{N_i}}$$

$\frac{(N_i + g_i - 1)^{N_i + g_i - 1}}{(g_i - 1)^{g_i - 1} N_i^{N_i}}$

$$\ln B = \sum_i \left[(g_i + N_i) \ln (g_i + N_i) - g_i \ln g_i - N_i \ln N_i \right]$$

zahtjev extr.: $\delta \ln B = 0$ $\delta N = 0 / \alpha$ $\delta U = 0 / \beta$

$N = \sum_i N_i$ $U = \sum_i N_i E_i$

$0 = \sum_i \delta N_i$ $0 = \sum_i E_i \delta N_i$

$$\delta (\ln B + \alpha N - \beta U) = 0$$

$$\delta \ln B = \sum_i \left\{ \sum_j \frac{\partial}{\partial N_j} \left[(g_i + N_i) \ln (g_i + N_i) \right] \delta N_j + \sum_j \frac{\partial}{\partial N_j} \left[-N_i \ln N_i \right] \delta N_j \right\}$$

$$= \sum_i \left\{ \ln (g_i + N_i)\, \delta N_i + \frac{g_i + N_i}{g_i + N_i} \delta N_i - \ln N_i\, \delta N_i - \frac{N_i}{N_i} \delta N_i \right\}$$

$$= \sum_i \left\{ \ln (g_i + N_i) + 1 - \ln N_i - 1 \right\} \delta N_i$$

$$\sum_i \left[\ln (g_i + N_i) - \ln N_i - \alpha - \beta E_i \right] \delta N_i = 0$$

$\forall i$ - proizv. varijacije

originalno (KB) Ideo ⇒

$$\ln (g_i + N_i) - \ln N_i - \alpha - \beta E_i = 0$$

$g_i + N_i = N_i\, e^{\alpha + \beta E_i}$ $g_i = N_i \left(e^{\alpha + \beta E_i} - 1\right)$

točnije:

$N_i = \frac{g_i - 1}{e^{\alpha + \beta E_i} - 1}$ *) ⇒

$$N_i = \frac{g_i}{e^{\alpha + \beta E_i} - 1}$$

Bose-ova raspodjela

→ populacija i-tog energ. nivoa

$$g_i = \frac{N_i}{g_i} = \frac{1}{e^{\alpha+\beta E_i} - 1}$$

- molekule gotovo svih plinova imaju celobrojan spin

$$dN = V \cdot \frac{4\pi p^2 dp}{h^3} \cdot \frac{1}{e^{\alpha+\beta E} - 1}$$

- Lagrange-ovi multiplikatori α, β odredjuju se preko uvjeta po kojima su uvedeni.

→ fizički smisao: $g_i > 0 \Rightarrow e^{\alpha+\beta E_{min}} \geq 1$

izvan djelovanja vanjskog polja $U=0$ $E = E_K \Rightarrow E_{min} = 0$

$$\Rightarrow e^{\alpha} \geq 1 \qquad \alpha \geq 0$$

- formalno očuvanje broja čestica za $\alpha = 0$, jer $\sum_i N_i = N \mid \cdot \alpha$ je nepotrebno uvesti ako broj čestica nije očuvan

Fotoni, fononi

- broj čestica nije sačuvan $\alpha = 0$

$E = \hbar\omega$ $\beta = \frac{1}{KT}$

$$N_i = \frac{g_i}{e^{\beta E_i} - 1} \Rightarrow g(\omega) = \frac{1}{e^{\frac{\hbar\omega}{KT}} - 1}$$

Planck-ova raspodjela
spec. slučaj Bose-Einstein-ove

Supek I 338.

- odaberimo kocku volum. V i impulsni prostor između $p, p+dp$.

⇒ broj elem. ćelija - kvantnih stanja u tom području

$$dg = g_i = 2V \cdot \frac{4\pi p^2 dp}{h^3}$$

, faktor 2 dobiti zbog dva smjera polarizacije vala

⇒ broj kvanata svjetlosti u intervalu dp

$$dN = 2V \frac{4\pi p^2 dp}{h^3} \cdot \frac{1}{e^{\beta E} - 1} \qquad E = \hbar\omega \quad p = \frac{\hbar\omega}{c} = \frac{h}{\lambda}$$

$$dN = \frac{V \cdot \omega^2 d\omega}{\pi^2 c^3} \cdot \frac{1}{e^{\frac{\hbar\omega}{KT}} - 1}$$

- broj čestica (kvanata) svjetlosti energije $\hbar\omega$

⇒ energija koja pada na interval frekvencija $d\omega$

$$u_\omega d\omega = \hbar\omega \cdot dN = V \frac{\hbar\omega^3 d\omega}{\pi^2 c^3} \cdot \frac{1}{e^{\frac{\hbar\omega}{KT}} - 1}$$

- time smo izveli Planck-ov zakon za čisto korpuskularnog shvaćanja. Kvalizam vala i čestice proizlazi dakle dubokim činom prirode, da se osnovni zakoni mogu dobiti pokazati ni korpuskularne ni

Fermioni

Pauli-ev princip → V kvantno stanje sadrži največ 1 čestico
spin $s = 1/2, 3/2, \ldots$

0| |0|0| | |0

$\Rightarrow$ $\underline{g_i \geq N_i}$ N_i - polnih celic
$g_i - N_i$ - praznih celic

$\underbrace{g_1\, g_2\, g_4 \cdots g_{i-1}\, g_i}_{N_i}$

poglavje (xx) $\Rightarrow$ $B_i = C_{g_i}^{N_i} = \binom{g_i}{N_i}$

$$B = \prod_i \frac{g_i!}{N_i!\,(g_i - N_i)!} \overset{\substack{g_i \gg 1 \\ N_i \gg 1}}{=} \prod_i \frac{g_i^{g_i}}{N_i^{N_i}\,(g_i - N_i)^{g_i - N_i}}$$

$$\ln B = \sum_i \left[-g_i \ln g_i - N_i \ln N_i - (g_i - N_i) \ln (g_i - N_i) \right]$$

$$\delta \ln B = \sum_i \left\{ \sum_j \frac{\partial}{\partial N_j} \left[-N_i \ln N_i \right] \delta N_j + \sum_j \frac{\partial}{\partial N_j} \left[-(g_i - N_i) \ln (g_i - N_i) \right] \delta N_j \right\} =$$

$$= \sum_i \left\{ -\ln N_i - \frac{N_i}{N_i} + \ln (g_i - N_i) - \frac{(g_i - N_i)(-1)}{(g_i - N_i)} \right\} \delta N_i = \sum_i \left\{ -\ln N_i + \ln (g_i - N_i) \right\} \delta N_i$$

- najverjetnejša razporeditev

$$\delta \left(\ln B - \alpha N - \beta U \right) = 0$$

$$\sum_i \left[\ln \frac{g_i - N_i}{N_i} - \alpha - \beta E_i \right] \delta N_i = 0$$

orig. (B) $\Rightarrow$ $\ln \frac{g_i - N_i}{N_i} - \alpha - \beta E_i = 0 \quad \forall i$

$\frac{g_i - N_i}{N_i} = e^{\alpha + \beta E_i}$

$\frac{g_i}{N_i} - 1 = e^{\alpha + \beta E_i}$

$\Rightarrow$ $\underline{N_i = \frac{g_i}{e^{\alpha + \beta E_i} + 1}}$

1926
Fermi-Diracova razporeditev

populacija: $\underline{\eta_i = \frac{1}{e^{\alpha + \beta E_i} + 1}}$

Bose-Einstein-ova statistika

[Jednake čestice ne možemo međusobno (individualno) razlikovati

cjelobrojan spin $s = 0, 1, ..$

$\Rightarrow$ otpada mogućnost rasporeda i^{tih} čestica na energetske nivoe (u smislu njihovog prirustva u nekom i-tom nivou) i dobivamo novih načina razmještaja (numeriranih čestica, jer ih sad nemamo pravo numerirati), već je neki nivo okarakteriziran po broju razmještaja nekog broja čestica na ćelije unutar tog nivoa pali stalno vodeći računa da je svejedno koje su čestice u ćeliji, već je samo bitno koliko ih je

(*) $\overset{1}{g_1}\overset{2}{g_1}\overset{3}{g_1}\overset{4}{g_2}\overset{5}{g_2}\overset{6}{g_4}\overset{7}{g_4} \cdots g_{i-1}^{N_i-1} g_i^{N_i}$

(**) $g_1\,123\;g_2\,45\;g_3\,g_4\,67 \cdots g_{i-1}\,(N_i-3)(N_i-2)\,g_i\,(N_i-1)\,N_i$

$1,2,3 \in g_1 \quad 4,5 \in g_2$

(*) $\Rightarrow$ Kombinacije s ponavljanjem od g_i elem. N_i-tog reda

$$\bar{C}_{g_i}^{N_i} = \binom{g_i+N_i-1}{N_i} = \frac{g_i\,(g_i+N_i-1)!}{g_i!\,N_i!} > \frac{g_i^{N_i}}{N_i!}$$

tj. ćelije bi nesamo kao predstavnici, a ne još i njihove permutacije u položaju što bi davalo razmještaje istog broja, ali različitih čestica u nekoj ćeliji

(**) $\Rightarrow$ $\dfrac{g_i\,(g_i+N_i-1)!}{g_i!\,N_i!}$ $\rightarrow$ ne $(g_i+N_i)!$ jer na početak nesmije doći broj (čestica) već ćelija

$\rightarrow$ permutacije čestica ne dovode nova mjesta jer ih nemamo (zbog) različitih

$\rightarrow$ ćelije međusobno razne prave pa permutacije njihove ne daju nova stalan raspored ćelija

$\rightarrow$ bilo koji raspored N_i čestica na g_i ćelija ali samo količinski (ne individualno)

$$\Rightarrow \quad \mathcal{B} = \prod_i \frac{g_i\,(g_i+N_i-1)!}{g_i!\,N_i!} = \prod_i \frac{(g_i+N_i-1)!}{(g_i-1)!\,N_i!}$$

$\sum_i \varepsilon_i N_i = U \qquad \sum_i N_i = N$ nezavisnih čestica

Fermi-eva statistika

(elektroni)

$\mathcal{F}$ - jednake čestice se ne mogu međusobno (individualno) razlikovati

polucijeli spin $s = 1/2$ $\Rightarrow$ 2° **Pauljev princip** - u jednom kvantnom stanju može biti samo jedna čestica ($s=1/2$) - elektron

------ E_i: N_i; g_i ćelija

$\Rightarrow$ $\underline{N_i \leq g_i}$

(*) $g_1^{\,1}\; g_2^{\,2}\; g_4^{\,3} \cdots g_{i-1}\; g_i^{\,N_i}$

(**) $\underline{g_1\,1}\;\underline{g_2\,2}\;g_3\;\underline{g_4\,3}\cdots\underline{g_{i-1}\,N_{i-1}}\;\underline{g_i\,N_i}$

(*) $\Rightarrow$ Kombinacije bez ponavljanja od g_i - elem. N_i - tog reda

$$C_{g_i}^{N_i} = \binom{g_i}{N_i} = \frac{g_i\cdot(g_i-N_i+1)}{N_i!} = \frac{g_i!}{(g_i-N_i)!\,N_i!}$$

$= 1$ za $N_i = g_i$

ćelije bitne samo kao pretinci, a ne još njihovo permutacije u položaju (u prirodnom poretku) što bi dovelo razmještaje istog broja, ali različitih čestica u poj. ćelijama

(**) $\Rightarrow$ $\dfrac{g_i!}{N_i!\,(g_i-N_i)!}$

$g_i!$ - broj permutacija svih ćelija

$N_i!$ - broj permutacija praznih ćelija - ne dobivamo nova raspodjela

$(g_i-N_i)!$ broj permutacija punih ćelija (različ. čestice u istim ćelijama) što s obzirom na 1° ne daje nikakva nova

$\Rightarrow$ $\underline{B = \prod_i \frac{g_i!}{(g_i-N_i)!\,N_i}}$

papar (*)

$p = \frac{h}{\lambda}$ $\quad Q = \frac{2\pi}{\lambda}$ $\Rightarrow \vec{p} = \hbar \vec{Q}$ $\quad k = \frac{1}{\lambda}$ $\quad Q = 2\pi \cdot k$

$Q = \frac{2\pi \cdot \nu}{c} = \frac{\omega}{c}$

valno brojenje stanja:

$u(\vec{r}) = A e^{i\vec{Q}\cdot\vec{r}}$ ravni val

→ Kutija periodičnosti: L_1, L_2, L_3

(ne zahtijeva da na rubovima valna fja. iščezava, već zahtjev periodičnosti) Sipek 317

$$A e^{i[Q_x(x+L_1)+Q_y\cdot(y+L_2)+Q_z\cdot(z+L_3)]} = A e^{i(Q_x\cdot x + Q_y\cdot y + Q_z\cdot z)}$$

$\Rightarrow Q_x L_1 = 2\pi n_1$ $\quad L_1, L_2, L_3$ postaju veliki $\Rightarrow Q_x, Q_y, Q_z$ quasikontinuir. varijable

$$Q_x = \frac{2\pi}{L_1}\cdot n_1 \quad Q_y = \frac{2\pi}{L_2}\cdot n_2 \quad Q_z = \frac{2\pi}{L_3}\cdot n_3$$

$n_1 = 1,2,3,\ldots$ $\quad n_2 = 1,2,\ldots$ $\quad n_3 = 1,2,3,\ldots$

broj stanja tj. ravnih valova $B = n_1 n_2 n_3$

$$dB = dn_1 dn_2 dn_3 = \frac{L_1 L_2 L_3}{(2\pi)^3} dQ_x\, dQ_y\, dQ_z$$

- to je broj ravnih valova između Q_x $Q_x + dQ_x$, Q_y $Q_y + dQ_y$, ...

→ broj stanja (valova) u intervalu energije dE (ili valnog vektora $d\vec{Q}$)

$$dB = \frac{L_1 L_2 L_3}{(2\pi)^3} 4\pi Q^2 dQ = \frac{V}{(2\pi)^3}\cdot 4\pi Q^2 dQ$$

$Q = \frac{\omega}{c} / \cdot 2\pi$

$k = \frac{\nu}{c}$

$$dB = \frac{V}{(2\pi)^3 c^3}\cdot 4\pi\omega^2 d\omega \quad \text{ili} \quad dB = \frac{V}{h^3} 4\pi p^2 dp$$

$p = \frac{h}{2\pi} Q$ $\quad \frac{L_1 L_2 L_3}{(2\pi)^3}\cdot 4\pi \frac{(2\pi)^3}{h^3} p^2 dp$

Korpuskularno valno titranje

$$\sum_i \varepsilon_i \rightarrow \int \frac{d\phi}{h^3} = \frac{V}{h^3} \int 4\pi p^2 dp$$

$$\Rightarrow d\varepsilon_i = dB = \frac{V}{h^3} 4\pi p^2 dp$$

→ Kod fotona i fonona dolazi još sumacija po polarizacijama

$$\sum_\sigma \cdot \sum_i \varepsilon_i \rightarrow 2 \int \frac{d\phi}{h^3} \quad \text{fotoni}$$

$$3 \int \frac{d\phi}{h^3} \quad \text{fononi}$$

→ općenito kod drugih čestica koje posjeduju spin S

$$\sum_\sigma \sum_i \varepsilon_i \rightarrow (2S+1) \int \frac{d\phi}{h^3}$$

napomena!!!

zapravo $\sum_i \varepsilon_i$ sve obuhvaća, pa i $\sum_\sigma \sum_i \varepsilon_i$

Veza s klasičnom statistikom

$$g_i = \frac{N_i}{g_i} = \frac{1}{e^{\alpha+\beta E_i} \pm 1}$$

fermioni
bozoni

$e^{\alpha+\beta E_{min}} \gg 1 \Rightarrow g_i = e^{-\alpha} \cdot e^{-\beta E_i}$ Boltzmann-ova raspodjela

→ specijalno: $U=0 \quad E_{min} = E_{k\,min} = 0$

$\Rightarrow e^{\alpha} \gg 1$

Šipek II 339.
za plinove kod normalnih temp. $\alpha \gg 0$
- molekule plina sekundarnim kontinuirano pomiču prema višim energijama i u tom slučaju nemamo potrebe uzimati diskretnost (ali ona olakšava pregled) - to je bitna razlika prema kvantnoj teoriji

Veza α & β s t-din. veličinama

$$\delta(\ln B - \alpha N - \beta U) = 0 \quad /\cdot K$$

Idvo (20)
- općenito izvedeno iz zahtjeva da se entropije zbrajaju, a t-din. vjerojatnosti množe (bez obzira na raspodjelu)

$$S = k_1 \ln B_{max} \quad (*) \quad k_1 = K$$ - Boltz. konst.

(21) Idvo provjereno za Boltzm. raspo.
postepeno dovođ energije plinu - godovo-ravnotežne promjene tako se mogla primjeniti Boltz. rasp.
→ analogna provjera iza ove raspod.: !!!

→ kao orig.!! na (56) godovo-ravnotežnim procesom mijenjamo N & U

$$\delta S = K\alpha \delta N + K\beta \delta U$$

$$K\alpha = \left(\frac{\partial S}{\partial N}\right)_{U,V} \qquad K\beta = \left(\frac{\partial S}{\partial U}\right)_{N,V}$$ - volumen

!tab.

*)

$S_m - S = K \ln \frac{B_m}{B}$

$\frac{B_m}{B} = e^{\frac{\Delta S}{K}}$

T-dim. sistem (idealni) – u kojem se mijenja broj čestica (propusne stijene)

$$V, N, T, P, U, S$$

aditivnost ↔ ekstenzivne veličine

- ukupni volumen $V = N v$ ← volumen koji otpada na 1 česticu — $\delta V = N\delta v + v\delta N$
- ukupna entropija $S = N \cdot s$ — $\delta S = N\delta s + s\delta N$
- ukupna energija umd. $U = N u$ — $\delta U = N\delta u + u\delta N$

v, s, u – mjerju svojstva 1 čestice

→ **Osnovna t-dim. relacija za 1 česticu**

$\delta' Q = \delta u + P\delta v$ & $\delta' Q = T\delta s$

I z.t.d. $\delta U = \delta' Q - \delta' A = \delta' Q - P\delta V$

II z.t.d. $\delta' Q = T\delta S$

$$\boxed{T\delta s = \delta u + P\delta v}$$

$$T\,\frac{\delta S - s\delta N}{N} = \frac{\delta U - u\delta N}{N} + P\,\frac{\delta V - v\delta N}{N} \quad / N$$

$$\Rightarrow \quad \boxed{T\delta S = \delta U + P\delta V - (u + Pv - Ts)\delta N}$$

- opisuje sistem u t-dim ravnoteži za odredit. broj čestica

- osnovna t-dim. relacija proširena na sisteme gdje se mijenja broj čestica

napomena !!!
u I dijelu za zrač. crnog tijela $G = 0 \Rightarrow$ ne ∃ odr. broja fotona

$F = U - TS$
$H = U + PV$
$G = H - TS$ } $G = U + PV - TS = F + PV$

→ Napišimo Gibbs-ov potencijal: (*)

$$G = U + PV - TS = Nu + PNv - TNs = N(u + Pv - Ts)$$

⇒ ono Gibbs-ov potenc. 1 čestice što ima aditivno svojstvo svedeno na 1 česticu

po analogiji:

def! $\boxed{\mu = u + Pv - Ts}$

Kemijski potencijal ili Gibbs-ova fja. za 1 česticu

$$\Rightarrow \quad \boxed{G = N\mu}$$

→ **Osnovna t-dim. relacija glasi:**

$$\delta S_{(U,V,N)} = \frac{1}{T}\delta U + \frac{P}{T}\delta V - \frac{\mu}{T}\delta N \quad i)$$

$U(V,T,P)$

- možemo pisati i diferencijale ali počeli smo s varijacijama

$$\Rightarrow \quad \frac{1}{T} = \left(\frac{\partial S}{\partial U}\right)_{V,N} = k\beta \qquad -\frac{\mu}{T} = \left(\frac{\partial S}{\partial N}\right)_{U,V} = k\alpha \qquad **)$$

*) & **) $\Rightarrow$

$$\alpha = -\frac{\mu}{kT} \qquad \beta = \frac{1}{kT}$$

isto vrijednosti za sve tri statistike

← pozvano od ranije

$g_i = \frac{1}{e^{\alpha+\beta E_i}+1}$

$$g_i = \frac{1}{e^{\frac{E_i-\mu}{kT}} \pm 1}$$

fermioni
bozoni

$g_i > 0 \Rightarrow e^{\alpha+\beta E_{min}} \geq 1 \quad U=0 \Rightarrow E_{min}=0 \Rightarrow e^{\alpha} \geq 1$

Bozoni: $e^{\alpha} \geq 1 \Rightarrow \alpha \geq 0 \Rightarrow \mu \leq 0$

$e^{\alpha+\beta E_i} \gg 1 \quad e^{\alpha+\beta E_{min}} \gg 1 \quad U=0 \quad E_{min}=0$

Kvant. stat. → Klas. stat. $e^{\alpha} \gg 1 \Rightarrow e^{-\beta\mu} \gg 1 \qquad e^{\beta\mu} \ll 1$

E_p za $U=0$ tj. $E=E_k$

T-din. ravnoteža - dva zatvorena sustava u t-din. ravnoteži: u smislu spojimo

odranije: ponovo u t-din. ravnoteži ako P, T iste, tada neće doći do promjene S zatvorenog sustava

može i diferencijal

$S = S_1 + S_2 \qquad \delta S = \delta S_1 + \delta S_2 = \frac{\delta U_1 + P_1 \delta V_1 - \mu_1 \delta N_1}{T_1} + \frac{\delta U_2 + P_2 \delta V_2 - \mu_2 \delta N_2}{T_2} \quad (*)$

const $\begin{cases} V = V_1 + V_2 & \Rightarrow \delta V_2 = -\delta V_1 \\ N = N_1 + N_2 & \Rightarrow \delta N_2 = -\delta N_1 \\ U = U_1 + U_2 & \Rightarrow \delta U_2 = -\delta U_1 \end{cases}$

što jedan sistem izgubi dobije drugi, što ne mora biti za entropiju tj. dalje $S = S_1 + S_2 = \text{const.}$

→ zahtjev: - t. din. ravnot. u smislu ne mijenjanja entropije

$$0 = \delta S = \delta U_1 \left(\frac{1}{T_1} - \frac{1}{T_2}\right) + \delta V_1 \left(\frac{P_1}{T_1} - \frac{P_2}{T_2}\right) - \delta N_1 \left(\frac{\mu_1}{T_1} - \frac{\mu_2}{T_2}\right)$$

zbog nezavisnosti: $U_1, V_1, N_1 \Rightarrow$ nezav. $\delta U_1, \delta V_1, \delta N_1$

$$\Rightarrow \quad T_2 = T_1 \qquad P_2 = P_1 \qquad \mu_2 = \mu_1$$

- dodatni zahtjev

bitno: za razumijevanje rada tranzistora - fizika čvrstog stanja

Mikro kanonski : $N=\text{const}$, $H=E=\text{const}$ $\quad S(H) = A\cdot\delta(H-E)$

Kanonski : $T=\text{const}$, $N=\text{const}$ $\quad S(H) = A\,e^{-\frac{H}{KT}}$

Velikokanonski sistem (potencijal) $\rightarrow N \neq \text{const.}$

Bozoni

str (53)

$$\ln B = \sum_i \left[(g_i+N_i)\ln(g_i+N_i) - g_i \ln g_i - N_i \ln N_i \right]$$

$\delta \ln B = 0 \Rightarrow (\ln B)_{max}$

$$= \sum_i \left[g_i \ln \frac{g_i+N_i}{g_i} + N_i \ln \frac{g_i+N_i}{N_i} \right]$$

$\ln(1+g_i)$ $\qquad$ $\ln(1+\frac{1}{g_i})$

$$g_i = \frac{N_i}{g_i} = \frac{1}{e^x-1} \qquad x = \frac{E_i-\mu}{KT}$$

$$1+g_i = \frac{e^x-1+1}{e^x-1} = \frac{e^x}{e^x-1} = \frac{1}{1-e^x} \qquad 1+\frac{1}{g_i} = 1+e^x-1 = e^x$$

$$(\ln B)_{max} = \ln B = -\sum_i g_i \ln\left[1-e^{\frac{\mu-E_i}{KT}}\right] + \underbrace{\sum_i \frac{N_i E_i - \mu N_i}{KT}}_{\frac{U-\mu N}{KT}}$$

$$\nu = \frac{\mu}{KT} = \beta\mu$$

$$\Rightarrow \ln B = \underbrace{-\sum_i g_i \ln\left[1-e^{\nu-\beta E_i}\right]}_{\Omega} + \beta U - \nu N$$

$S = k_1 \ln B$ (*) str (55)

$$S = K(\Omega + \beta U - \nu N) \qquad iii)$$

$$\Omega = -\sum_i g_i \ln\left[1-e^{\nu-\beta E_i}\right]$$

velikokanonski potencijal za bozone

originalno!! (drugačiji nalaženja $\beta = \frac{1}{k_1 T}$)

→ zatvoreni sistem polako zagrijavamo dovodeći mu toplinu tj:

možemo pisati i diferencijale $\delta U = \delta' Q = T\delta S \neq 0 \quad \delta' A = 0$ tako da sistem prolazi kroz niz ravnotežnih stanja, pa tada možemo primijeniti raspodjelu u ∀ od tih trenutaka (kao da se u njima raspodjela ne mijenja)

Neka je još sistem zatvoren $N = \sum_i N_i = \text{const.}$

$$\ln B = -\sum_i g_i \ln(1-e^x) + \sum_i N_i \ln e^x \qquad g_i = \frac{N_i}{g_i} = \frac{1}{e^x-1} \qquad x = \alpha + \beta E_i$$

$$= -\sum_i g_i \ln(1-e^{\alpha+\beta E_i}) + \alpha N + \beta U$$

varijacija po broju čestica na pojedinoj energ. nivou

& Supek I (34) $\delta U = \sum_i E_i \delta N_i - P\delta V$

$$\left.\begin{array}{l} \delta \ln B = \beta \delta U = \beta \delta' Q = \beta \cdot T \delta S \\ \text{označimo } S = k_1 \ln B \end{array}\right\} \Rightarrow \beta \cdot T = \frac{1}{k_1} \Rightarrow \beta = \frac{1}{k_1 T}$$

$k_1 = K$

→ primjenom Boltzmann-ove raspodjele na idealni plin str (24e) dobiva se jba. idealnog plina $PV = NKT \overset{nR}{\Rightarrow} k_1 = \frac{R}{N} = 1{,}38\cdot 10^{-16}$ ergs

– analogno i za ostale

→ odredujemo pravila za određivanje fizičkih veličina

– usporedivanje s t-din. zapisom (da bi našli fizičko značenje Ω)

iii) ⇒ $\delta S = k(\delta\Omega + \beta\delta U + U\delta\beta - \nu\delta N - N\delta\nu)$ $\quad \nu = \beta\mu$

$= \left(\frac{1}{kT}\delta U + \frac{P}{kT}\delta V - \frac{\mu}{kT}\delta N\right)\cdot k$

i) ⇒ $\delta S = k(\beta\delta U + \beta P\delta V - \nu\delta N)$

$$\Rightarrow \quad \delta\Omega = \beta P\delta V - U\delta\beta + N\delta\nu$$

$$P = kT\left(\frac{\partial\Omega}{\partial V}\right)_{\beta,\nu} \qquad U = -\left(\frac{\partial\Omega}{\partial\beta}\right)_{V,\nu} \qquad N = \left(\frac{\partial\Omega}{\partial\nu}\right)_{V,\beta}$$

(ii) bozoni

jba. stanja — ukupna energija — broj čestica

specijalno: zadržit sve ponavljanje izraze

Fermioni

str 54

$$\ln B = \sum_i \left[g_i \ln g_i - N_i \ln N_i - (g_i - N_i)\ln(g_i - N_i)\right]$$

$$= \sum_i \left[g_i \ln \frac{g_i}{g_i - N_i} + N_i \ln \frac{g_i - N_i}{N_i}\right]$$

$\frac{1}{1 - \frac{N_i}{g_i}}$ $\qquad \frac{g_i}{N_i} - 1$

$$\frac{N_i}{g_i} = \frac{1}{e^x + 1} \qquad x = \alpha + \beta E_i = \frac{E_i - \mu}{kT}$$

$\frac{1}{1 - g_i} = \frac{1}{1 - \frac{1}{e^x+1}} = \frac{e^x+1}{e^x+1-1} = 1 + e^{-x}$ $\qquad \frac{1}{g_i} - 1 = e^x + 1 - 1 = e^x$

$$(\ln B)_{max} = \sum_i g_i \ln\left(1 + e^{\frac{\mu - E_i}{kT}}\right) + \sum_i N_i \frac{E_i - \mu}{kT}$$

$$\Rightarrow (\ln B)_{max} = \underbrace{\sum_i g_i \ln\left[1 + e^{\nu - \beta E_i}\right]}_{\Omega} + \beta U - \nu N \qquad (*)$$

(*) str 55

$$S = k(\Omega + \beta U - \nu N) \qquad \text{iii)}$$

$$\Omega = \sum_i g_i \ln\left[1 + e^{\nu - \beta E_i}\right]$$

veličina kanonski potencijal za fermione

originalno ?!! (kao i na 56)

varijacija po broju čestica na pojedinom nivou: $\delta \ln B = \beta\delta U = \beta\cdot\delta Q = \beta\cdot T\delta S$

$S = k_1 \ln B_{max}$ $\Rightarrow \beta\cdot T = \frac{1}{k_1} \Rightarrow \beta = \frac{1}{k_1 T}$

→ iiii) je identično po obliku iii) te koristeći i) ponovno dobijemo relacije (i) za ju. stanja, ukupnu energiju i ukupan broj čestica samo s tom razlikom da je:

(i) sadrži sve prethodne relacije kao spec. slučaj

$$\Omega = \pm \sum_i g_i \ln\left(1 \pm e^{\nu - \beta E_i}\right) \qquad \begin{matrix} + \\ - \end{matrix} \begin{matrix} \text{Fermioni} \\ \text{Bozoni} \end{matrix}$$

→ provjerimo relaciju $U = -\left(\frac{\partial \Omega}{\partial \beta}\right)_{V,\nu}$ & $N = \left(\frac{\partial \Omega}{\partial \nu}\right)_{\beta,V}$

$\alpha = -\frac{\mu}{KT} = -\nu$

$$-\left(\frac{\partial \Omega}{\partial \beta}\right)_{V,\nu} = -\left\{ \pm \sum_i g_i \frac{\pm e^{\nu - \beta E_i} \cdot (-E_i)}{1 \pm e^{\nu - \beta E_i}} \right\} = \sum_i g_i E_i \frac{1}{e^{-\nu + \beta E_i} \pm 1} = \sum_i E_i \underbrace{\frac{g_i}{e^{\alpha + \beta E_i} \pm 1}}_{N_i}$$

$$= \sum_i E_i N_i = U$$

$$\left(\frac{\partial \Omega}{\partial \nu}\right)_{\beta,V} = \pm \sum_i g_i \frac{\pm e^{\nu - \beta E_i}}{1 \pm e^{\nu - \beta E_i}} = \sum_i \frac{g_i}{e^{-\nu + \beta E_i} \pm 1} = \sum_i \underbrace{\frac{g_i}{e^{\alpha + \beta E_i} \pm 1}}_{N_i} =$$

$$= \sum_i N_i = N$$

→ **Specijalno:**

Fotoni, fononi - quasi čestice čiji broj nije očuvan

$\alpha = -\frac{\mu}{KT}$ ② $T = 0$

$\alpha = 0 \Rightarrow \mu = 0, \nu = 0 \qquad E_i = \hbar\omega$

$E_{N_i} = N_i E_i = N_i \hbar\omega$

$\bar{E}(\omega) = E_i \cdot \frac{1}{e^{\beta E_i} - 1} = N(\omega) \cdot \hbar\omega$ broj fotona frekv. ω

- bozoni

$p = \frac{h}{\lambda} = \frac{h\nu}{c}$

$\sum_i g_i \to \int \frac{d\phi}{h^3} = \frac{V}{h^3} \int d^3p \, 4\pi p^2 dp = \frac{4\pi V}{h^3} \int p^2 dp$

$$\Omega = -\sum_{\vec{p},G} \ln\left(1 - e^{\nu - \beta\hbar\omega}\right)_{\nu=0}$$

sumacija po polarizaciji, pasmu izostavili faktor degeneracije g_i (koji je jednak 2)

$$S = K(\Omega + \beta U - \nu N)$$

$\Omega = \frac{S}{K} - \frac{1}{KT} U = -\frac{1}{KT}(\underbrace{U - TS}_{F})$ ($n = 0$)

$$\Rightarrow \quad F = -KT\Omega = KT \sum_{\vec{p},G} \ln\left(1 - e^{\nu - \beta\hbar\omega}\right)_{\nu=0}$$

$\sum_{\vec{p},G}$ ustvari $\sum_{\vec{p}} \sum_{G}$

- osnovna relacija pri proučavanju fotonskih i fononskih sistema

Veza s Klasičnom statistikom

$$g_i = \frac{N_i}{g_i} = \frac{1}{e^{\alpha+\beta E_i} \pm 1}$$ Fermioni, Bozoni $\qquad \alpha = -\frac{\mu}{kT} = -\nu$

$e^{\alpha+\beta E_{min}} \gg 1 \qquad U=0 \Rightarrow E_{min}=0 \Rightarrow e^{\alpha} \gg 1 \qquad e^{\nu} = e^{-\alpha} \ll 1$

→ **Klasični limes velikokanonskog potencijala**

(*) $e^{\nu} \ll 1 \Leftarrow e^{\nu-\beta E_i} = e^{-(\alpha+\beta E_i)} \ll 1 \Leftarrow$ zahtjev $e^{\alpha+\beta E_i} \gg 1 \quad \forall i$

$$\Omega = \pm \sum_i g_i \ln\left(1 \pm \underbrace{e^{\nu-\beta E_i}}_{x \ll 1}\right) \qquad \ln(1\pm x) = \pm\left[\pm x \mp x^2 \dots\right] \overset{x\ll 1}{\approx} \pm x$$

$$\Omega \approx \pm \sum_i \pm g_i e^{\nu-\beta E_i}$$

$$\Omega = e^{\nu} \underbrace{\sum_i g_i e^{-\beta E_i}}_{Z}$$

Z - particijska fja. jedne čestice

$$N = \left(\frac{\partial \Omega}{\partial \nu}\right)_{V,\beta} = e^{\nu} \sum_i g_i e^{-\beta E_i} = e^{\nu} \cdot Z$$ novo

$$Z = z^N$$ - kad nema interakcije

$$\Rightarrow U = -\left(\frac{\partial \Omega}{\partial \beta}\right)_{V,\nu} = -e^{\nu}\left(\frac{\partial Z}{\partial \beta}\right)_{V,\nu} = -\frac{N}{Z}\left(\frac{\partial Z}{\partial \beta}\right)_{V,\nu} = -N\left(\frac{\partial \ln Z}{\partial \beta}\right)_{V,\nu}$$

općenito $F = -kT(\Omega - \nu N)$ $\overset{(*)}{\Rightarrow}$ uz $F = -NkT\ln z$

$$\Rightarrow U = \left(\frac{\partial \beta F}{\partial \beta}\right)_{V,\nu}$$

$\Omega = e^{\nu} Z = N \qquad e^{\nu} \ll 1 \Rightarrow \nu \ll 0$

$F = -NkT\left(\frac{\Omega}{N} - \nu\right) = -NkT(1-\nu) \overset{\nu\ll 0}{\approx} -NkT(-\nu)$

$\ln Z = \ln N - \nu \overset{\nu\ll 0}{\approx} -\nu \Rightarrow F = -NkT\ln Z$

$$P = kT\left(\frac{\partial \Omega}{\partial V}\right)_{\beta,\nu} = kTe^{\nu}\left(\frac{\partial Z}{\partial V}\right)_{\beta,\nu} = NkT\left(\frac{\partial \ln Z}{\partial V}\right)_{\beta,\nu} = -\left(\frac{\partial F}{\partial V}\right)_{\beta,\nu}$$ Maxwell-ova relacija

→ napomena!!! da je $F = -NkT\ln Z$ moguće dokazati usporedbom izraza za U sa odgovarajućim izrazima iz t-dinamike

$$U = -\left(\frac{\partial \ln Z^N}{\partial \beta}\right)_{V,\nu} \overset{Z^N = Z}{=} kT^2\left(\frac{\partial \ln Z}{\partial T}\right)_{V,\nu} = T\left[\left(\frac{\partial}{\partial T} kT\ln Z\right)_{V,\nu} - k\ln Z\right] = -kT\ln Z + T\left(\frac{\partial}{\partial T} kT\ln Z\right)_{V,\nu}$$

$\frac{\partial}{\partial \beta} = \frac{\partial}{\partial T}\frac{\partial T}{\partial \beta} \qquad \frac{\partial T}{\partial \beta} = \frac{1}{\partial \beta / \partial T} = -\frac{1}{k\beta^2}\frac{\partial}{\partial T} = -kT^2\frac{\partial}{\partial T}$

$S = -\left(\frac{\partial F}{\partial T}\right)_V \qquad U = F + T\left[-\left(\frac{\partial F}{\partial T}\right)_V\right] = F - T\left(\frac{\partial F}{\partial T}\right)_V$

$F = U - TS$

$dF = dU - TdS - SdT$

$= TdS - PdV - TdS - SdT$

$= -PdV - SdT$

ista struktura izraza

$\Rightarrow$

$$F = -kT\ln Z = -NkT\ln z$$

1-A idealni plin

$$\Omega = \pm \sum_{\text{bozoni}}^{\text{Fermioni}} \sum_i g_i \ln\left(1 \pm e^{\nu - \beta E_i}\right) \qquad \nu = \beta\cdot\mu$$

- kod translac. st. slobode $\sum \to \int$

jer nivoi energ. bliski: ΔE $T = 10^{-14}K$ kocka $a = 1cm$ $m = 10^{-23}g$

- kvantizac. energ. znači: nešto tak kod aps. nule

Ukupan broj kvantnih stanja

$$\sum_i g_i \to \frac{2S+1}{h^3}\int d\phi \; d^3\vec{r}\, d^3\vec{p} =$$

(fazni volumen; 3-transl. st. slobode)

S - spin čestice: $\vec{M} = S\,\hbar$ → $2S+1$ stanja; $\vec{M}$ & M_z kvant. brojevi

$$= \frac{2S+1}{h^3}\cdot V \int 4\pi p^2 dp$$

(za $U_{int} = 0$ pase kod idealnog plina može integrirati po koord.; polarni sustav)

- slobodna čestica $E = \frac{p^2}{2m}$ $\Rightarrow$ $p\,dp = m\,dE$

$p^2 dp = m\sqrt{2mE}\,dE$

$$= \frac{2S+1}{h^3}\cdot V \cdot \int_0^\infty 4\pi m\sqrt{2mE}\,dE = \int_0^\infty g(E)\,dE$$

$g(E)\,dE$ - broj stanja između $E, E+dE$

gustoća stanja

$$g(E) = \frac{2S+1}{h^3}\cdot 2\pi \cdot V (2m)^{3/2} E^{1/2}$$

$$\beta = \frac{1}{KT} \qquad t = \beta E \qquad dE = \beta^{-1}\,dt$$

$$E^{1/2} = \beta^{-1/2} t^{1/2}$$

$$\Omega = \pm \frac{2S+1}{h^3}\cdot 2\pi V \cdot \left(\frac{2m}{\beta}\right)^{3/2} \int_0^\infty \sqrt{t}\,\ln\left(1 \pm e^{\nu - t}\right) dt$$

(ne ovisi o β, niti V)

$$U = -\left(\frac{\partial \Omega}{\partial \beta}\right)_{V,\nu} = \frac{3}{2}\cdot\frac{1}{\beta}\,\Omega = \frac{3}{2}KT\,\Omega$$

$$P = KT\left(\frac{\partial \Omega}{\partial V}\right)_{\beta,\nu} = KT\cdot\frac{\Omega}{V}$$

$$U = \frac{3}{2}P\cdot V$$

isto vrijedi kao i u klas. stat. fizici

- za 1-A idealni plin gdje smo gledali translac. st. slobode

Klasični limes · Kvantne statistike

$$g_i = \frac{1}{e^{\frac{E_i-\mu}{kT}} \pm 1} = \frac{e^{\frac{\mu-E_i}{kT}}}{1 \pm e^{\frac{\mu}{kT}} \cdot e^{-\frac{E_i}{kT}}} = e^{\frac{\mu-E_i}{kT}} \left[1 \mp x + x^2 \mp x^3 \right]$$

($e^{\frac{\mu}{kT}} = x$, $e^{-\frac{E_i}{kT}} \leq 1$; bozoni; za $|x| < 1$)

$\alpha = -\frac{\mu}{kT}$ $\quad e^{\alpha+\beta E_i} \gg 1$ za $U=0 \Rightarrow E_{i_{min}} = 0$

$\Rightarrow e^{\alpha} \gg 1 \Rightarrow e^{\frac{\mu}{kT}} \ll 1$

Klas. limes za: $e^{-\frac{\mu}{kT}} = \alpha$

protp: $e^{-\frac{\mu}{kT}} > 1$ tj. $\mu < 0$ & za bozone uvjek $E_i > 0$

(fiz. smisao $g_i > 0 \Rightarrow e^{\alpha} \geq 1 \Rightarrow \alpha \geq 0 \Rightarrow \mu < 0$ per za bozone) nekad moguće i za fermione

$$g_i = e^{\frac{\mu-E_i}{kT}} \left[1 \mp e^{\frac{\mu-E_i}{kT}} + \dots \right]$$

(1 bozoni; $e^{\frac{\mu-E_i}{kT}}$ ↓ Kvantna korekcija)

→ Kvantna korekcija ne igra ulogu, ako je

*) $e^{\nu} \ll 1 \Leftarrow e^{\frac{\mu-E_i}{kT}} \ll 1 \ \forall i \Rightarrow e^{\frac{E_i-\mu}{kT}} \gg 1$

($\nu = \frac{\mu}{kT}$, $U=0 \Rightarrow E_{min}=0$)

što sino odmah mogli reći, međutim ovdje tražimo zahtjev na populaciju

$\Rightarrow g_i = \frac{N_i}{g_i} \ll 1$

drugi oblik zahtjeva: $(mkT)^{3/2} \frac{V}{N} \gg h^3$ $\Leftrightarrow$ $N_i \ll g_i$ *) - populacija mala → uvjet primjenjivosti klas. stat. fizike

- broj čestica u faznom prostoru << broja ćelija

- tako siromašan broj čestica tako da tek koja kvantna ćelija popunjena ⇒ nemamo potrebe voditi računa o kvant. meh. principu da jednake čestice nerazlikujemo

$$N = \sum N_i = \sum_i g_i \cdot g_i \quad \text{(idealni plin)} \quad \sum_i g_i \to \frac{2S+1}{h^3} \cdot 2\pi V (2mkT)^{3/2} \int_0^{\infty} \frac{\sqrt{t}\,dt}{e^{t-\nu} \pm 1}$$

($\frac{1}{2}\pi^{1/2} e^{\nu}$; $\beta(\mu=\nu) \approx e^{\nu} \int_0^{\infty} t^{1/2} e^{-t}\,dt$; $\Gamma(3/2) = \frac{1}{2}\sqrt{\pi}$; Koristimo *) zanemarivo $\forall i$ $e^{\frac{E_i-\mu}{kT}} \gg 1$)

$$e^{\nu} = \frac{Nh^3}{(2S+1)V(2\pi mkT)^{3/2}} = \frac{\lambda^3}{(2S+1)\frac{V}{N}} = a$$

(u Klas. izrazu ?; λ^3 – tipična Kvantna veličina; $\frac{V}{N}$ – tipična Klas. veličina; de Broglie $\lambda = \frac{h}{p} \approx \frac{h}{\sqrt{2m\pi kT}}$ ubacili Kvantni faktor)

a - faktor degeneracije

& *) $\Rightarrow$ $\frac{h^3}{\frac{V}{N}(mkT)^{3/2}} \ll 1$ **) $\Leftrightarrow$ *)

Klasični limes - ako $\hbar \to 0$ ili $T \to \infty$ $\frac{V}{N}$ veliko

$\Rightarrow \lambda \to 0$ mali kvantni efekti

$a \sim \frac{\lambda^3 \to 0}{\frac{V}{N}}$ isto malo

$\Rightarrow$

$\Leftarrow$ $a \ll 1$ Klasična statistika $\Leftrightarrow (mkT)^{3/2} \cdot \frac{V}{N} \gg \hbar^3$

$\Rightarrow$ $a \gg 1$ Kvantna statistika - degenerirani plin

pogledaj str 65

1) $\frac{N}{V} = 2{,}7 \cdot 10^{19}$ $T = 272\,K$ $s = 0$ $m = 10^{-23}\,g$

$\Rightarrow a = 2 \cdot 10^{-6}$

za plin kod norm. uvjeta vrijedi Klas. statistika

2) elektronski plin u metalu

$\frac{N}{V} = 5 \cdot 10^{22}$ $s = \frac{1}{2}$ $m = 9{,}1 \cdot 10^{-28}\,g$ $T = 300\,K$

$\Rightarrow a = 10^3 \gg 1$

visoko degenerirani plin

Toplinski kapacitet - samo translacioni st. slobode

- za boz. i fermi. raspodjelu na niskim temp. slaganje s III z.t.d. - Nernst

nezbog kvantizacije kao kod 2-A molek C_V^{rot}, titranja Kristal. rešetke već zahvaljujući novoj distribucionoj fji. - odnosno principu nerazlikovanja

| slučaj 1-A idealnog plina

provjeri $U = \frac{3}{2} kT \Omega$ $\Omega = \frac{1}{\hbar^3} \frac{2S+1}{2} 2\pi V \left(\frac{2m}{\beta}\right)^{3/2} \int_0^\infty \sqrt{t} \ln(1 \pm e^{\nu - t}) dt$

$(2mkT)^{3/2}$ ne ovisi o β, V

$C_V = \left(\frac{\partial U}{\partial T}\right)_V \sim \frac{\partial}{\partial T} (T)^{5/2} \sim \frac{5}{2} T^{3/2} \xrightarrow[T \to 0]{} 0$

$\Rightarrow$ dakle zbog kvantne stat. $\Rightarrow$ fja. raspodjele dakle da

i za translac st. slob. C_V iščezava za $T \to 0$

Idealni 1-A plin

Degenerirani sistem fermiona

$\alpha = -\frac{\mu}{KT}$ $\quad \nu = \beta\cdot\mu$

$\mu(T) \gg KT$ – uvjeta $a = e^{\nu} = e^{\frac{\mu}{KT}}$ degeneracija fermion. sustava $\Leftrightarrow a \gg 1$

idel. plin $\frac{\lambda^3}{(2S+1)\frac{V}{N}}$ $\quad \lambda = \frac{h}{\sqrt{2m\pi KT}}$ $\quad <1$

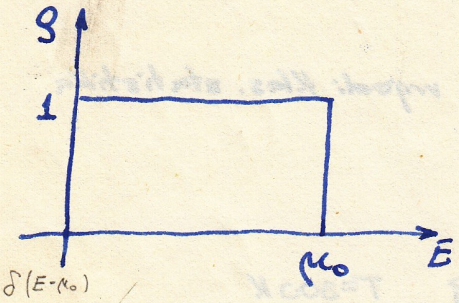
Sup. K II 341. granična energija

$\mu \gg KT \Leftrightarrow \mu_0 \gg KT \Leftrightarrow T \ll T_F = \frac{\mu_0}{K} \Rightarrow a \approx \left(\frac{T_F}{T}\right)^{3/2} \gg 1$ str. 65

a) potpuno degeneriran $T = 0°K$

Fermijeva fja. $\rightarrow$ $g = \frac{1}{e^{\frac{E-\mu}{KT}}+1} = \begin{cases} 1 & E < \mu_0 \\ 0 & E > \mu_0 \end{cases}$

energ kem potencijal



μ_0 – kem. potencijal apsol. nule

$\mu_0 = \mu(0)$ $\quad \mu = -KT\alpha \neq \mu(T)$

$\Rightarrow \lim_{\varepsilon\to 0} \frac{dg(E)}{dE} = -\delta(E-\mu_0)$

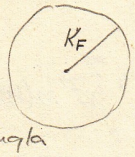
$\rightarrow$ jer $\lim_{T\to 0} g = \begin{cases} 0 & E > \mu_0 \\ 1 & E < \mu_0 \end{cases}$

$$-\frac{dg}{dE} = \delta(E-\mu_0) \quad \text{za } E > 0$$

$\rightarrow$ Fermionski sistem popunjava redom najniža energetska stanja – do μ_0 (posljedica Pauli-eva principa) na $T = 0$

tj. sve čestice ne mogu doći na najniže energetsko stanje, već u k-tom kvantnom stanju najviše 1 čestica

$\rightarrow$ u K-prostoru $\vec{K}_F$ – Fermijev valni vektor



Kugla

Fermijeva energija: $\mu_0 = \frac{\hbar^2 K_F^2}{2m}$

– " – brzina: $\vec{V}_F = \frac{\hbar \vec{K}_F}{m}$

– " – temperatura degener.: $T_F = \frac{\mu_0}{K}$

→ Kako Fermijeva energija μ_0 ovisi o koncentraciji čestica u sistemu

$$N = \sum_i N_i = \sum_i g_i \vartheta_i \qquad \sum_i g_i \to \int_0^\infty \frac{2S+1}{h^3} \cdot V \cdot 4\pi m \sqrt{2mE}\, dE$$

$$\Rightarrow N = \sum_i g_i \vartheta_i \to \int_0^\infty g(E)\,\vartheta(E)\,dE$$

za idealni plin gdje prom. translac. stupnji slobode gdjesu energ. nivoi gusti $\Rightarrow \Sigma \to \int$ $\quad g_i(E_i) \to g(E)$

$$N = \frac{2S+1}{h^3} \cdot 2\pi V (2m)^{3/2} \int_0^\infty \vartheta(E)\sqrt{E}\, dE$$

za $T=0$

$$\int_0^\infty \vartheta(E)\sqrt{E}\,dE = \int_0^{\mu_0} \sqrt{E}\,dE = \frac{1}{1+\frac{1}{2}} E^{3/2}\Big|_0^{\mu_0} = \frac{2}{3}\mu_0^{3/2}$$

$$\Rightarrow N = \frac{2S+1}{h^3} \cdot \frac{4\pi}{3} V (2m\mu_0)^{3/2}$$

$$\mu_0 = \left[\frac{3h^3 N}{4\pi V (2S+1)}\right]^{2/3} \cdot \frac{1}{2m}$$

→ Fermijeva energija raste s porastom koncentracije čestica i padom mase čestica

Kod $T=0$

idealni plin translacijski st. slobode gusti

$$U = \sum_i N_i E_i = \sum_i g_i \vartheta_i E_i \xrightarrow{} \int_0^\infty g(E)\cdot\vartheta(E)\,E\,dE \xrightarrow{T=0} \int_0^{\mu_0} g(E)\,E\,dE$$

$$U_0 = \frac{2S+1}{h^3} \cdot 2\pi V (2m)^{3/2} \int_0^{\mu_0} E^{3/2}\,dE = \frac{2}{5}\mu_0^{5/2} = N \cdot \frac{2}{5}\mu_0$$

$$\Rightarrow U_0 = \frac{3}{5} N \mu_0$$

→ prosječna energija jedne čestice na $T=0$ je $\frac{3}{5}$ Fermijeve energije

usporedimo: $\Rightarrow P_0 = \frac{2S+1}{h^3} \cdot \frac{4\pi}{5} (2m)^{3/2} \cdot \frac{2}{5}\mu_0^{5/2}$

str 57 $\Rightarrow U_0 = \frac{3}{2} P_0 V$

→ i na $T=0$ fermijev plin proizvodi neki tlak

- posljedica Paulijevog principa

- kao i svi kvantni efekti - povezano s h

$h \to 0$, ona $\to 0$

$$P_0 = \frac{2S+1}{h^3} \cdot \frac{8\pi}{15} (2m)^{3/2} \cdot (2m)^{-5/2} \left[\frac{3h^3 N}{4\pi V (2S+1)}\right]^{5/3} = \frac{(2S+1)8\pi}{15\cdot(2m)} \cdot \left[\frac{3N}{4\pi V (2S+1)}\right]^{5/3} \cdot h^2 \xrightarrow{h\to 0} 0$$

$\mu_0 \xrightarrow{h\to 0} 0$

$U_0 \xrightarrow{h\to 0} 0$

b) $T > 0$ $\quad \mu(T) \gg KT$ (i)

$S_i = \frac{1}{e^{\frac{E_i - \mu}{KT}} + 1}$ za idealni plin → translac. st. slobode - gusti do 10^{14} K

$$S(E) = \frac{1}{e^{\frac{E-\mu}{KT}} + 1}$$

$E = \mu \pm \Delta E \geq 0 \Rightarrow E \gg \mu$ za $\Delta E \gg$
$E \ll \mu$

$$S(\mu \pm \Delta E) = \frac{1}{e^{\pm\frac{\Delta E}{KT}} + 1}$$

$$S(\mu+\Delta E) + S(\mu-\Delta E) = \frac{1}{e^{\frac{\Delta E}{KT}}+1} + \frac{1}{e^{-\frac{\Delta E}{KT}}+1} = \frac{1}{e^{\frac{\Delta E}{KT}}+1} + \frac{e^{\frac{\Delta E}{KT}}}{1+e^{\frac{\Delta E}{KT}}} = 1$$

$$\Rightarrow S(\mu+\Delta E) + S(\mu-\Delta E) = 1$$

jer $\Delta E \geq 0$ $\quad \Delta E = 0 \Rightarrow S(\mu) = \frac{1}{2}$

→ za $\Delta E \gg KT \Rightarrow S \to 0$ za $+$ tj: $E \gg \mu$
$S \to 1$ za $-$ tj: $E \gg \mu$

→ što je T viša $S \to \begin{cases} 0 \\ 1 \end{cases}$ polaganje tj. Klja. je položenija

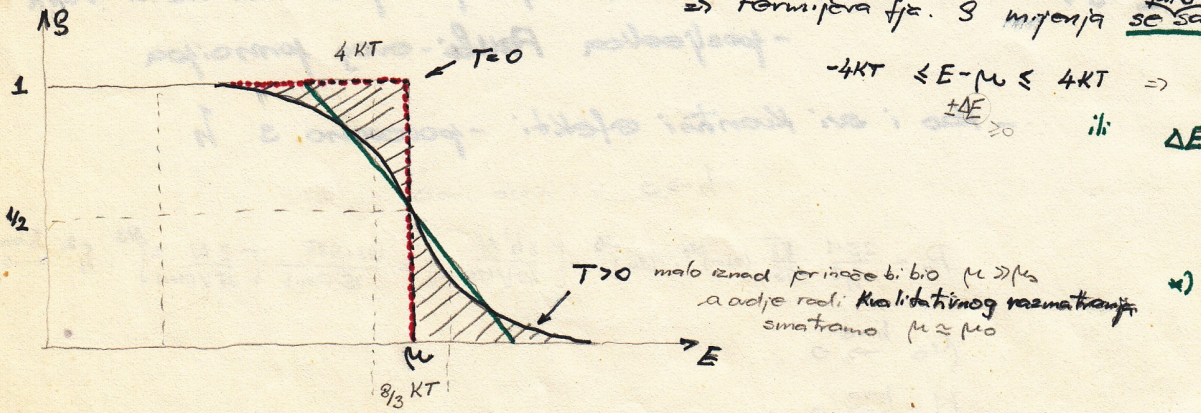
extremno za $T = 0$ Klja. potpuno strma

→ za $\Delta E \approx KT \Rightarrow$ promjena S između 1 & 0

(ii) $\Rightarrow \Delta E \approx KT \ll \mu(T)$ dakle, promjena S između 1 & 0 u uskom području oko μ

$\Rightarrow$ Fermijeva fja. S mijenja jako se samo u uskom području

$-4KT \leq E - \mu \leq 4KT \Rightarrow |E-\mu| \leq 4KT$
$\pm\Delta E \geq 0$ ili $\Delta E = |\Delta E| \leq 4KT$



malo iznad je mora biti $\mu \gg \mu_0$ (*)
a odje radi kvalitativnog razmatranja smatramo $\mu \approx \mu_0$

→ **Kvalitativno razmatranje**: - u blizini μ aprox. S ravnom kosom crtom

fizik. značenje - zagrijavanjem od 0 do T prelaze fermioni iz gornjeg prezarenog područja u donje → sistem prešao u pobuđeno stanje iznad Fermijeve energije $\mu_0 \approx \mu$ za $T > 0$ malo tj. termičkim pobuđenjem prelaze iznad tog nivoa u malom intervalu oko Fermijevog nivoa

→ **porast energije** - sistema je term. pobuđenjem energija poraste

$$\Delta U = N_{ef} \cdot KT$$ - prosječna energija tog reda veličine

↓ broj čestica koje su prešle u pobuđeno stanje i preuzele termički iznos KT

∞ površini trokuta $\frac{\frac{1}{2} 4KT}{2} = KT$

$$\frac{N_{ef}}{N} \simeq \frac{KT}{\mu_0} \quad (\sim KT,\ \sim \frac{1}{\mu_0}) \quad \Rightarrow \quad \Delta U \simeq N \cdot \frac{(KT)^2}{\mu_0} = N\mu_0 \left(\frac{KT}{\mu_0}\right)^2$$

poredu veličine

$$U_0 = \frac{3}{5} N\mu_0 \quad \Rightarrow \quad \Delta U \simeq U_0 \left(\frac{KT}{\mu_0}\right)^2$$

$\mu_0 \gg KT$ ⇒ term. pobuđenjem mali postotak čestica prešao u pobuđ. stanje

(*) ⇒ prirast energije $\ll$ nego u slučaju Klas. stat. fizike

$$U = U_0 + \Delta U = U_0 \left(1 + \frac{5}{3}\left(\frac{KT}{\mu_0}\right)^2\right) = U_0 + N\mu_0 \left(\frac{KT}{\mu_0}\right)^2$$

faktor reda veličine 1 $\ll 1$

$$\Rightarrow \quad C_v = \left(\frac{\partial U}{\partial T}\right)_V \simeq NK \cdot \frac{KT}{\mu_0} \quad (*) \quad \to 0 \quad \text{za } T \to 0$$

$\ll 1$

zadovoljen Nernst-ov tm.

Supek I 343.

→ specifična toplina elektronskog plina proporcionalna je temperaturi. Zaključak, ona je kod svih normalnih temperatura znatno manja od specifične topline kristala. No budući da spec. toplina kristala iščezava kao T^3, mora u blizini apsolutne nule prevladavati spec. toplina elektronskog plina. Takve fine crte u ponašanju spec. topline čvrstih tijela exp. su dosada pronađene.

→ **Korektan izvod**: Sommerfeld (1928)

→ ideja postupka pretpostavka

$$-\frac{dS}{dE} \approx \delta(E-\mu) \quad \text{i za } T>0$$

⇒ u integralima $\int_0^\infty P(E) \frac{dS}{dE} dE$ $P(E)$ razvijemo oko singulariteta μ

$P(E)$ ... $P(E)$

$\pm \Delta E$

$$E = \mu + (E-\mu)$$

integral po potencijama $\left(\frac{KT}{\mu}\right)^2$

Sommerfeld-ov razvoj - Fermioni

$$\frac{N_i}{g_i} = \mathcal{G}_i = \frac{1}{e^{\frac{E_i-\mu}{kT}}+1} \qquad N = \sum_i N_i = \sum_i g_i \mathcal{G}_i \qquad U = \sum_i N_i E_i = \sum_i g_i \mathcal{G}_i E_i$$

$$\varrho = \frac{2\pi}{\lambda} \qquad \vec{p} = \hbar\vec{\varrho} \qquad E = \frac{p^2}{2m} = \frac{\hbar^2\varrho^2}{2m} \qquad \varrho = \frac{\sqrt{2m}}{\hbar}\sqrt{E}$$

$$d\varrho = \frac{1}{2}\frac{\sqrt{2m}}{\hbar}E^{-1/2}dE$$

papir (2)

$$\sum_i g_i \to \int dB = \int dn = \frac{V}{(2\pi)^3}\int d^3\varrho = \frac{V}{8\pi^3}4\pi\int_0^\infty \varrho^2 d\varrho = \frac{V}{8\pi^3}\cdot 4\pi\cdot\frac{1}{2}\cdot\frac{(2m)^{3/2}}{\hbar^3}\int_0^\infty E^{1/2}dE$$

ili $= \frac{V}{\hbar^3}4\pi\int_0^\infty p^2 dp = \int_0^\infty \frac{V(2m)^{3/2}}{4\pi^2\hbar^3}\sqrt{E}\,dE$

→ **Karakterističan prijelaz na integral**

- za gusta stanja (kao transko. st. slob. do 10^{14} K)

$$f(E) \equiv \mathcal{G}(E) = \frac{1}{e^{\frac{E-\mu}{kT}}+1}$$ Fermi-ova fja. raspodjele

broj stanja:

$$\varrho = \frac{2\pi}{\lambda} \Rightarrow \vec{p} = \hbar\vec{\varrho}$$

Oznake na Vježbama → $dn \equiv dB = d^3n = \frac{V}{(2\pi)^3}\underbrace{d^3\varrho}_{d^3K'''} = \frac{V}{2\pi^2}\varrho^2 d\varrho$

za 1 česticu $E = \frac{\hbar^2\varrho^2}{2m}$ $\varrho = \frac{1}{\hbar}\sqrt{2mE}$

$$d\varrho = \frac{1}{\hbar}\sqrt{2m}\,E^{-1/2}\cdot\frac{1}{2}dE$$

$$dn \equiv dB = \frac{V(2m)^{3/2}}{4\pi^2\cdot\hbar^3}\sqrt{E}\,dE$$

def: $D(E) \equiv \frac{dn}{dE} \equiv g(E) = \frac{dB}{dE} = \frac{V(2m)^{3/2}}{4\pi^2\hbar^3}\cdot\sqrt{E}$

Kao na (59) samo $g(E) = \frac{2S+1}{8\pi^3\cdot\hbar^3}\cdot 2\pi V(2m)^{3/2}E^{1/2}$

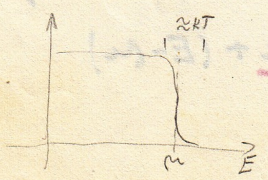
$$\Rightarrow \sum_i g_i[\,] \to \int_0^\infty [\,]g(E)dE$$

$$N = \sum_i N_i = \sum_i g_i \mathcal{G}_i \to \int_0^\infty \mathcal{G}(E)\,g(E)dE \qquad U = \sum_i N_i E_i = \sum_i g_i \mathcal{G}_i E_i \to \int_0^\infty \mathcal{G}(E)\,E\,g(E)dE$$

$$\Rightarrow N = \int_0^\infty \mathcal{G}(E)\,g(E)dE \qquad U = \int_0^\infty \mathcal{G}(E)\cdot\frac{dn}{dE}dE$$

broj stanja na interval $E, E+dE$

$$U = \int_0^\infty \mathcal{G}(E)\,E\,g(E)dE \qquad U = \int \mathcal{G}(E)E\frac{dn}{dE}dE$$



→ sistem Fermiona se sabija u kuglu u energetskom prostoru

→ $I(E) = g(E) \sim E^{1/2}$ ... pa ovo pare deriv. druge f/e $\frac{2}{3}\frac{d}{dE}\left(E^{3/2}\right)^{\varphi(E)}$

→ općenito mrijed.: $E = \mu + (E-\mu)$

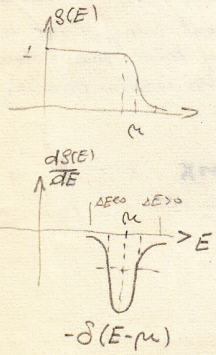
$$J = -\int_0^\infty \varphi(E)\frac{\partial f(E)}{\partial E}dE = \varphi(\mu) + 2\sum_{n=1}^{\infty}(kT)^{2n}\varphi^{(2n)}(\mu)\left(1-2^{1-2n}\right)\zeta(2n) \quad (*)$$

pretp. $\varphi(0) = 0$ npr. $\frac{\partial \varphi(E)}{\partial E} = g(E)$ ili $E\,g(E)$ $\quad f(E) = g(E) = \frac{1}{e^{\frac{E-\mu}{kT}}+1} \Rightarrow f(\infty) = 0$

$$\int_0^\infty g(E)\cdot\underbrace{\frac{\partial \varphi}{\partial E}}_{dv}dE = \underbrace{[g(E)\cdot\varphi(E)]_0^\infty}_{=0} - \int_0^\infty \varphi(E)\frac{\partial g}{\partial E}dE$$

dokaz:

$$J = -\int_0^\infty \varphi(E)\frac{\partial f(E,\nu)}{\partial E}dE = -\int_0^\infty \varphi(E)\frac{\partial g}{\partial E}dE$$



$\Delta E = E-\mu$

$$\frac{\partial g}{\partial E} = \frac{-\beta e^{\beta(E-\mu)}}{\left[e^{\beta(E-\mu)}+1\right]^2} = \frac{-\beta}{\left(e^{\beta(E-\mu)}+1\right)\left(e^{-\beta(E-\mu)}+1\right)} = \frac{-\beta}{\left(e^{\beta\Delta E}+1\right)\left(e^{-\beta\Delta E}+1\right)} =$$

$$= \frac{-\beta}{2+e^{\beta\Delta E}+e^{-\beta\Delta E}} = \frac{-\beta}{2+\sum_{n=0}^{\infty}\frac{1}{n!}\left[(\beta\Delta E)^n+(-\beta\Delta E)^n\right]} = \frac{-\beta}{2+2\sum_{n=0}^{\infty}\frac{1}{(2n)!}(\beta\Delta E)^{2n}} \approx -\delta(E-\mu)$$

→ oštro $\frac{\partial g}{\partial E}$ sim. f/a, parna f/a. s obzirom na ΔE ... za usporedbu $|\beta\Delta E| \gg 1$ dovoljno je da prismo

$\beta\Delta E \gg 1 \Rightarrow \frac{\partial g}{\partial E} \approx -\beta e^{-\beta\Delta E} \to 0$ i)

$$\frac{1}{2} = \frac{\left(\frac{\partial g}{\partial E}\right)_{|\Delta E|>0}}{\left(\frac{\partial g}{\partial E}\right)_{\Delta E=0}} = \frac{\frac{-\beta}{2+e^{\beta\Delta E}+e^{-\beta\Delta E}}}{-\frac{\beta}{4}} \quad X = e^{\beta\Delta E} \Rightarrow X^2-6X+1=0 \Rightarrow |\beta\Delta E| \approx 1$$

$X_1X_2 = 1$, $X_{1,2} = \frac{6\pm\sqrt{32}}{2}$

$\Delta E \approx kT \overset{(*)}{\ll} \mu$ iii)

i) & iii) ⇒ iiii) $\frac{\partial g}{\partial E}$ sliči $-\delta(E-\mu)$

$$\varphi(E) = \varphi(\mu+(E-\mu)) = \sum_{n=0}^{\infty}\frac{\varphi^{(n)}(\mu)}{n!}(E-\mu)^n$$

$\mu \gg kT \Rightarrow \beta\mu \gg 1$

$$J = -\sum_{n=0}^{\infty}\frac{\varphi^{(n)}(\mu)}{n!}\int_0^\infty (E-\mu)^n\frac{dg}{dE}dE \approx -\sum_{n=0}^{\infty}\frac{\varphi^{(n)}(\mu)}{n!}\int_{-\infty}^{\infty}(E-\mu)^n\frac{dg}{dE}dE$$

jer već za $E=0 \Rightarrow \Delta E = -\mu$

$$\left(\frac{\partial g}{\partial E}\right)_{E=0} = \frac{-\beta}{2+e^{-\beta\mu}+e^{\beta\mu}} \overset{(*)}{\approx} -\frac{1}{kTe^{\beta\mu}} \overset{(*)}{\to} 0$$

→ dalje $\int_0^\infty (E-\mu)^n\frac{dg}{dE}dE \overset{(*)}{\approx} \int_{-\infty}^{\infty}(E-\mu)^n\frac{dg}{dE}dE = \int_{-\infty}^{\infty}\underbrace{(\Delta E)^n}_{\text{neparna f/a. s obzirom na } \mu \text{ za } n\text{-neparan}}\underbrace{\frac{dg}{dE}}_{\text{parna f/a. od } \Delta E \text{ s obzirom na } \mu}(\Delta E) = 0$ za n-neparan

$$\Rightarrow J = -\sum_{n=0}^{\infty}\frac{\varphi^{(2n)}(\mu)}{(2n)!}\int_{-\infty}^{\infty}(E-\mu)^{2n}\frac{dg}{dE}dE = \varphi(\mu) - \sum_{n=1}^{\infty}\frac{\varphi^{(2n)}(\mu)}{(2n)!}\int_{-\infty}^{\infty}(E-\mu)^{2n}\frac{dg}{dE}dE$$

$n=0$ $\int_{-\infty}^{\infty}\frac{dg}{dE}dE = \int_{-\infty}^{\infty}-\delta(E-\mu)dE = -1$ ili $\int_{-\infty}^{\infty}\frac{dg}{dE}dE = g(E)\Big|_{-\infty}^{\infty} = g(\infty)-g(-\infty) = -1$ iiii)

sa faktorom 2, jer podintegralna fja $(E-\mu)^{2l}\frac{dg}{dE}$ je simetrična s pram točke μ, a ne 0, gdje ova već približno iščezava

$$(*) \Rightarrow \quad J = \varphi(\mu) - 2\sum_{l=1}^{\infty} \frac{\varphi^{(2l)}(\mu)}{(2l)!} \underbrace{\int_{\mu}^{\infty} (E-\mu)^{2l} \frac{dg}{dE}\, dE}_{J_1(2l)}$$

$$x = \frac{E-\mu}{KT} \qquad E-\mu = (KT)x \qquad \frac{dg}{dE} = \frac{-\beta}{2+e^{x}+e^{-x}} \qquad g(E) = \frac{1}{e^{x}+1}$$

$$\beta(E-\mu) = x$$

$E=\mu \Rightarrow x=0$

$E=\infty \Rightarrow x=\infty$ $\qquad \frac{d}{dE} = \frac{dx}{dE}\frac{d}{dx} = \frac{1}{KT}\frac{d}{dx} \qquad dE = KT\cdot dx$

$$\Rightarrow \underline{J_1} = (KT)^{2l}\int_0^{\infty} x^{2l}\underbrace{\frac{dg}{dx}}_{dv}\cdot dx$$

$$= (KT)^{2l}\left(x^{2l}\, g(E)\Big|_0^{\infty} - (KT)^{2l}\cdot 2l\int_0^{\infty}\frac{x^{2l-1}}{e^{x}+1}\,dx\right)$$

$g(E)_{x=\infty}=0$

$$= -(KT)^{2l}\cdot 2l\int_0^{\infty} x^{2l-1}\cdot\frac{e^{-x}}{1+e^{-x}}\,dx$$

za $\mu \le E \le \infty$ $\quad \int_{\mu}^{\infty} dE$

$\Rightarrow 0 \le x \le \infty$ $\quad \int_0^{\infty} dx$

$\Rightarrow e^{-x} < 1$ za $0 < x \le \infty$ osim za $x=0$

međutim za odredeni integral nije bitno da li u toj rubnoj točci $x=0$ možemo fju razviti ili ne, ako u svim ostalim možemo

$$\frac{e^{-x}}{1+e^{-x}} = \frac{e^{-x}}{1-(-e^{-x})} = e^{-x}\sum_{m=0}^{\infty}(-e^{-x})^{m} = \sum_{m=0}^{\infty}(-1)^{m}e^{-(m+1)x} \qquad m'=m+1$$

$$= -(KT)^{2l}\cdot 2l\sum_{m=0}^{\infty}(-1)^{m}\int_0^{\infty} x^{2l-1}\cdot e^{-(m+1)x}\,dx$$

$$t = mx \qquad x = \frac{1}{m}t \qquad dx = \frac{1}{m}dt$$

$$= -(KT)^{2l}\cdot 2l\sum_{m=1}^{\infty}(-1)^{m-1}\int_0^{\infty} x^{2l-1}\cdot e^{-mx}\,dx$$

$$\frac{1}{m^{2l-1}}\cdot\frac{1}{m}\int_0^{\infty} t^{2l-1}e^{-t}\,dt$$

$$= -(KT)^{2l}\cdot 2l\sum_{m=1}^{\infty}\frac{(-1)^{m-1}}{m^{2l}}\cdot\underbrace{\int_0^{\infty} t^{2l-1}e^{-t}\,dt}_{\Gamma(2l)=(2l-1)!}$$

$$= -(KT)^{2l}\cdot(2l)!\sum_{m=1}^{\infty}\frac{(-1)^{m-1}}{m^{2l}} = \eta$$

$m = 1,2,3,\ldots$

$m = 2m'$

$$\sum_{m=1}^{\infty}\frac{(-1)^{m-1}}{m^{n}} = \sum_{m=1}^{\infty}\frac{(-1)^{m+1}}{m^{n}} = \sum_{m\text{-neparan}}^{\infty}\frac{1}{m^{n}} + \sum_{m\text{-paran}}^{\infty}\frac{(-1)}{m^{n}} = \sum_{m=1}^{\infty}\frac{1}{m^{n}} - 2\sum_{m\text{-paran}}\frac{1}{m^{n}}$$

$$= \sum_{m=1}^{\infty}\frac{1}{m^{n}} - \frac{2}{2^{n}}\sum_{m=1}^{\infty}\frac{1}{m^{n}} = \left(1-2^{1-n}\right)\sum_{m=1}^{\infty}\frac{1}{m^{n}}$$

$$J_1 = -(KT)^{2l}\cdot(2l)!\left(1-2^{1-2l}\right)\underbrace{\sum_{m=1}^{\infty}\frac{1}{m^{2l}}}_{=\zeta(2l)}$$

Riemann-ova fja.

$\zeta(2) = \frac{\pi^2}{6}$

$\zeta(4) = \frac{\pi^4}{90}$

$$\Rightarrow J = \varphi(\mu) + 2\sum_{l=1}^{\infty}(KT)^{2l}\left(1-2^{1-2l}\right)\zeta(2l)\,\varphi^{(2l)}(\mu)$$

$$J = \varphi(\mu) + 2\left\{(KT)^{2}\left(1-\tfrac{1}{2}\right)\zeta(2)\varphi^{(2)}(\mu) + (KT)^{4}\left(1-2^{-3}\right)\zeta(4)\varphi^{(4)}(\mu) + \ldots\right.$$

$$J = \varphi(\mu) + \frac{\pi^2}{6}(KT)^{2}\varphi^{(2)}(\mu) + \frac{7\pi^4}{360}(KT)^{4}\varphi^{(4)}(\mu) + \ldots$$

za fizps. strukturu

geriranako $\frac{KT}{\mu} \ll 1$

zak. kod normalnih temp. pa kamoli kod niskih

$\Rightarrow$

$\varphi(0)=0$

$$(*)\quad \int_0^\infty g(E)\cdot\frac{\partial\varphi(E)}{\partial E}dE = -\int_0^\infty \varphi(E)\frac{\partial g}{\partial E}dE = \varphi(\mu)+2\sum_{n=1}^{\infty}\left(1-\frac{1}{2^{2n-1}}\right)\zeta(2n)(kT)^{2n}\varphi^{(2n)}(\mu)$$

$$= \varphi(\mu)+\frac{\pi^2}{6}(kT)^2\varphi^{(2)}(\mu)+\frac{7\pi^4}{360}(kT)^4\varphi^{(4)}(\mu)+\dots$$

London-Lifšic (Statist. fizika) $\rightarrow f(E)=\frac{\partial\varphi}{\partial E}$ $\Rightarrow$ $\int_0^\mu f(E)dE = \varphi(\mu)-\varphi(0)=\varphi(\mu)$ ($\varphi(0)=0$)

& $f'(\mu)=\varphi^{(2)}(\mu)$ itd.

$$\int_0^\infty \frac{f(E)dE}{e^{\frac{E-\mu}{kT}}+1} = \int_0^\mu f(E)dE + \frac{\pi^2}{6}(kT)^2 f'(\mu)+\frac{7\pi^4}{360}(kT)^4 f'''(\mu)+\dots$$

$\rightarrow$ $g(E) = \underbrace{\frac{(2S+1)V(2m)^{3/2}}{4\pi^2\hbar^3}}_{=\gamma} E^{1/2} = \gamma\cdot E^{1/2}$ $(*)'$

Vježbe (21) & (22)

$$N = \frac{(2S+1)V(2m)^{3/2}}{4\pi^2\hbar^3}\cdot\frac{2}{3}\mu^{3/2}\left[1+\frac{\pi^2}{8}\left(\frac{kT}{\mu}\right)^2+\dots\right] \Rightarrow N=\frac{2}{3}\gamma\mu_0^{3/2}$$

$$U = \frac{(2S+1)V(2m)^{3/2}}{4\pi^2\hbar^3}\cdot\frac{2}{5}\mu^{5/2}\left[1+\frac{5\pi^2}{8}\left(\frac{kT}{\mu}\right)^2+\dots\right] \Rightarrow U_0=\frac{2}{5}\gamma\mu_0^{5/2}=\frac{3}{5}N\mu_0$$

$$\mu(T) = \mu_0\left[1-\frac{\pi^2}{12}\left(\frac{kT}{\mu_0}\right)^2+\dots\right]$$ dobivamo korištenjem relacije za N

$$\Rightarrow U = \frac{3}{5}N\mu_0\left[1+\frac{5\pi^2}{12}\left(\frac{kT}{\mu_0}\right)^2+\dots\right]$$

$$C_V = \frac{N\pi^2k^2}{2\mu_0}\cdot T \rightarrow 0 \quad \text{za } T\rightarrow 0$$

$dS=\frac{dQ}{T}=C_V dT$

$$S=\int\frac{C_V}{T}dT = C_V T+\text{const.} \rightarrow 0 \quad \text{za } T\rightarrow 0$$

zadovoljen Nernst-ov tm.

Degenerirani sistem bozona

- bitne razlike od fermiona u blizini $T=0$
- najniže energetsko stanje → sve čestice na osnovnom energ. nivou

u prostoru valnog vektora → kondenzacija na osnovnom energ. nivou

Einstein-ova kondenzacija (1925)

→ kvalitativna procjena

$$\int_0^\infty \frac{\sqrt{E}}{e^{\frac{E-\mu}{kT}}-1}\,dE \qquad \frac{E}{kT}=t \qquad \sqrt{E}=(kT)^{1/2}\,t^{1/2} \qquad dE=(kT)\,t$$

$$N=\frac{(2s+1)V(2m)^{3/2}}{4\pi^2\hbar^3}(kT)^{3/2}\int_0^\infty \frac{\sqrt{t}}{e^{t-\nu}-1}\,dt$$

za bozonski sistem fiz. smisao $\delta_i(E)>0 \Rightarrow$ za $U=0$ $E_{min}=0 \Rightarrow e^{-\nu}>1 \Rightarrow e^{\nu}<1$

$\frac{1}{1-\frac{\nu-t}{e}}$ $\quad \frac{E-\mu}{kT}>0 \Rightarrow E>\mu \Rightarrow \nu-t<0$

$$\int_0^\infty \frac{\sqrt{t}\,dt}{e^{t-\nu}-1}=\int_0^\infty e^{\nu-t}\cdot\sqrt{t}\left[1+e^{\nu-t}+e^{2(\nu-t)}+\dots\right]dt=$$

$e^{\nu-t}=e^{\nu}\cdot e^{-t}$ ($\nu<1$, $t>0$) — za bozone $E_i>0$

$$=\sum_{n=1}^\infty e^{n\nu}\cdot\int_0^\infty e^{-nt}\cdot\sqrt{t}\,dt \qquad nt=u,\ dt=\frac{1}{n}du$$

$$\frac{1}{n}\cdot\frac{1}{\sqrt{n}}\int_0^\infty u^{1/2}e^{-u}\,du \qquad \Gamma\left(\tfrac{3}{2}\right)=\frac{\sqrt{\pi}}{2}$$

$$=\frac{\sqrt{\pi}}{2}\sum_{n=1}^\infty \frac{e^{n\nu}}{n^{3/2}}$$

$$N=\underbrace{\frac{(2s+1)V}{4\pi^2\hbar^3}(2mkT)^{3/2}\cdot\frac{\sqrt{\pi}}{2}}_{(1)}\ \underbrace{\sum_{n=1}^\infty \frac{e^{n\nu}}{n^{3/2}}}_{(2)}$$

$\nu=\frac{\mu}{kT} \qquad \mu<0 \rightarrow e^{-\frac{n|\mu|}{kT}}$

→ snižavamo T sistema, a N, V ostaju konstantni:

$\Rightarrow$ (1) ↘ a (2) ↗ $\quad e^{-\frac{n|\mu|}{kT}}$ bi padao, kad se μ ne bi mijenjao s T

→ budući $N=\text{const} \Rightarrow$ za (1) ↘ $\Rightarrow$ (2) ↗ $\Rightarrow |\mu(T)|$ ↘ za T ↘

i to brže nego za T

kažemo $\mu(T)\sim T^2$

jer T ↘ $|\mu|$ ↘

$\Rightarrow \mu_{max}=0$ za $T=T_c$

tada $N=\frac{(2s+1)V}{4\pi^2\cdot\hbar^3}(2mkT_c)^{3/2}\cdot\frac{\sqrt{\pi}}{2}\cdot\zeta\left(\frac{3}{2}\right)=\frac{(2s+1)V}{8\pi^2\cdot\pi\cdot\hbar^3}(2mkT_c)^{3/2}\cdot\pi^{3/2}\zeta\left(\frac{3}{2}\right)$

$(2)_{max} \rightarrow \zeta\left(\frac{3}{2}\right)=\sum_{n=1}^\infty \frac{1}{n^{3/2}}=2{,}612$

za $T < T_c$ (1) se ne može više povećati, tj. ne može se više vršiti kompenzacija s (1)

- ispod T_c učinili loše što se tiče matematika
- matematička pogreška $\Sigma \to \int$

ako $T \searrow$ ⇒ sve veći broj čestica pada na osnovno energetsko stanje - koje u integralu nije uključeno!

$$g(E) \sim \sqrt{E}$$

$$N = \int_0^\infty g(E) \cdot \mathcal{G}(E) dE$$ → time nismo uključili čestice na osnovnom energetskom stanju $E=0$ $N_i = g_i \cdot \mathcal{G}_i$

prije to nije bila velika pogreška zbog Pauljevog principa

$T \searrow$ sve veći broj č. na $E=0$, treba posebno obračunati taj doprinos č. za $E=0$

⇒ $$N = N_0 + N_p$$

N_0: broj čestica na osnovnom stanju → bozonska distribucijska fja. za $E=0$

N_p: broj čestica na pobuđenim energ. stanjima

$g_0 = 2S+1$

$N_0 = g_0 \cdot \mathcal{G}_0$ $\qquad \mathcal{G}_0 = \dfrac{1}{e^{-\frac{\mu}{kT}} - 1}$

$$N_0 = \frac{2S+1}{e^{-\frac{\mu}{kT}} - 1}$$

$$N_p = \frac{(2S+1)V}{4\pi^2 \hbar^3} (2mkT)^{3/2} \cdot \frac{\sqrt{\pi}}{2} \cdot \zeta(3/2) = N \left(\frac{T}{T_c}\right)^{3/2} \quad \text{za } T < T_c$$

- dakle znatan broj bozona na $E=0$ - Kondenzacija!

- dok za $T > T_c$ samo neznatan broj bozona na osnovnom energ. (Kv.) stanju

- mogli bismo „proračunati" velikokanonski potencijal Ω

→ ovdje je od interesa C_v

$$T_c = \frac{1}{2\pi m k} \left[\frac{N h^3}{(2S+1) V \cdot 2{,}612} \right]^{2/3}$$

- odgovara Fermijevoj temperaturi: $T_F = \frac{\mu_0}{k} = \frac{1}{2mk} \left[\frac{3Nh^3}{4\pi V (2S+1)} \right]^{2/3}$ str. 6

faktor $a = e^{\nu} \approx \left(\frac{T_F}{T}\right)^{3/2}$

- $T \gg T_c$ klasični limes str. 59 $\quad a = e^{\nu} = \dfrac{Nh^3}{(2S+1) V (2\pi m k)^{3/2} T^{3/2}} = \left(\frac{T_c}{T}\right)^{3/2} \ll 1$ tj. $N_i \ll g_i$

- $T \ll T_c$ degenerirani bozonski plin $\quad a = e^{\nu} = \left(\frac{T_c}{T}\right)^{3/2} \gg 1$

Procjenimo T_c : 1-A plin idealn.

$\frac{N}{V} = 10^{+20}$ $\quad m = 10^{-24}\,g$ $\quad s = 0$ $\quad \Rightarrow \quad T_c = 0{,}5\,K$

Kondenzacija nastupa na vrlo niskim temp.

→ $T < T_c$ → sve veći broj čestica na osn. stanju $E=0$, pa one ne daju doprinose U, P

Ukupna energija :

$$U = N_p \cdot \underbrace{KT}_{\text{u prosjeku}} \sim T^{5/2}$$

rad relativno na 1 česticu

$$\Rightarrow \quad C_v \sim T^{3/2}$$

$$S = \int \frac{C_v}{T}\,dT \sim T^{3/2} + S_0$$

integrac. konst.

→ akademski interes : dobili smo model idealnog plina koji se slaže s Nernst-ovim teoremom

Primjene :

→ **Bozoni** -

He_4 - tekući helij → izotopi He_3 He_4 razlikuju se u svojim statist. obilježjima

He_4	He_3
2e	2e
2P	2P
2N	1N
$S=0$	$S=1/2$
↓	↓
sim. valna fja.	asim. valna fja.
⇓	⇓
Bose-Einstein.	Fermi-Dirac

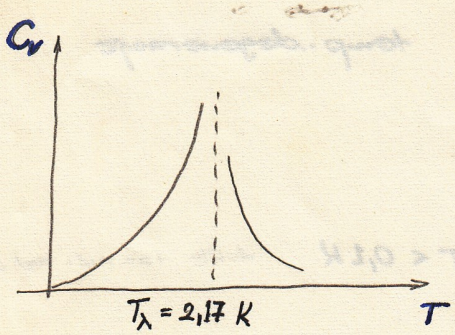
- ostaje spin neutrona
- Paulijev princip

He_4 prelazi u tekući na $T = 4\,K$

↓

u grubo aprox. primjena ovih razmatranja na tekući He_4

Einstein-ova temp. T_c jako nisko



← λ prijelaz

za $T < T_\lambda$ dvije komponente: normalna
superfluidna $S=0$ & koef. viskoznosti ≈ 0

London - tumačenje λ prijelaza s Einstein-ovom kondenzacijom

normalna komponenta - čestice koje nisu prešle na osnovno stanje, tj. koje su još na pobuđenim stanjima

superfluidna komponenta - čestice koje su prešle na osnovno stanje

$T < T_c = 0{,}5\ K$ $\quad C_v \sim T^3$ ($T^{3/2}$ za idealni plin, a u tekućini je za očekivati sile interakcije)

→ **Fermioni** -

skupovi s velikim μ $\quad \mu = \mu_0 \left[1 - \frac{\pi^2}{12}\left(\frac{kT}{\mu_0}\right)^2 + \dots\right]$ gdje $\mu_0 = \left[\frac{3\hbar^3 N}{4\pi V(2S+1)}\right]^{2/3} \cdot \frac{1}{2m}$

1) Nukleoni - velika kon. nukleona u jezgri

$\frac{N}{V} = 10^{38}$ $\quad T_F = \frac{\mu_0}{k} \Rightarrow T_F = 10^{11}\ K$

2) Bijeli patuljci (plazma) $\quad \varrho = 10^5 - 10^7\ g/cm^3$

elektroni i jezgre He

$m = 9{,}1 \cdot 10^{-28}$ $\quad \frac{N}{V} = 10^{30} \Rightarrow T_F = 10^9\ K$ $\quad$ brzine $\simeq c$

relativističke relacije

3) He_3 - tekući - exp.

$S = 1/2$

sadašnja granica exp.

- do temperature 0,005 K nema λ prijelaza

Što je i za očekivati jer He_3 nije bozon → u skladu s Londonovim tumačenjem preko Einst. kondenzacije

$\frac{N}{V} = 16 \cdot 10^{22}$ $m = 3 \cdot 167 \cdot 10^{-24}$ $\Rightarrow$ $T_F = 5\,K$ temp. degeneracije

- kao plin $C_V \sim T$ očekivati kod 1 K (možda još)

ali to vrijedi (exp.) zal za $T < 0{,}1\,K$ dakle izaći vrl. velične

- fakuć. privlačne sile snižavaju Fermijeve energ. nivoe, pa i T_F

4) Elektroni u metalu

$\frac{N}{V} = 5 \cdot 10^{22}$ $T_F \simeq 5 \cdot 10^4 K$ vrlo visoka temp. degeneracija

metal tali kod 10^3 K

→ u zbiljskom intervalu čistog metala - el. plin vrsto degeneriran

jer $T \ll T_F = \frac{\mu_0}{K}$ $\Rightarrow$ $\mu = \mu_0\left[1 - \frac{\pi^2}{12}\left(\frac{KT}{\mu_0}\right)^2\right]$ $\mu > \mu_0 \gg KT$ - a to je uvjet za degeneraciju

$\Rightarrow$ $C_V \sim T$ zapravo $C_V = \frac{\pi^2}{2}\left(\frac{KT}{\mu_0}\right)(NK)$ - po klas. statistici

i znatno manji ($\frac{1}{1}$) od onog po Klas. statistici NK

→ objašnjen slabi doprinos elektrona topl. kapacitetu

orig!!! - ne preko kvantiz. energ (kao kod rotacije i oscil. zanemarivanjem st. slobode) već za transl. st. slobode idealnog el. plina preko nove distribucione fje.

→ situacija se mijenja na niskim temp.

Debye teor. $C_V^{rešetke} \sim T^3$ $T \ll \Theta$

pa se zbog T^3 dobiva doprinos el. na niskim temp.